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APPROXIMATE SOLUTIONS OF A NON-LINEAR FIELD EQUATION

by

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled Approximate Solutions of a Non-Linear Field Equation, submitted by William B. Strickfaden, in partial fulfillment of the requirements for the degree of Master of Science.

ABSTRACT

A brief account is given of a proposal by Dr. H. Schiff for a six-vector unitary field theory. The static approximation to the equations is found and is the basis for the remaining part of the thesis.

The nature of the spherically symmetric solutions of the static equation is discussed; most of the results being taken from a paper by Finkelstein, et al., and it is shown that in addition to a continuum of solutions asymptotic to $\pm\sqrt{3}$, there exist discrete solutions, asymptotic to zero, which could represent neutral bosons.

The interaction potential energy between the discrete solutions as given by an approximate expression is discussed. The analytic interaction energy curves computed by Teshima are studied in detail for the existence of quantum mechanical and classical bound states.

The static equation is shown to be the Euler equation of a certain Lagrangian. Several integral relationships satisfied by the solutions are proved and on this basis a variational method which always gives upper bounds to the energy is formulated.

The variational method is used to calculate spherically symmetric solutions and it is shown that these solutions do approximate the spherically symmetric solutions obtained by numerical integration. A solution of odd parity is sought by means of

the variational method with the conclusion that no single particle solution of odd parity exists.

ACKNOWLEDGEMENTS

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I. Introduction

The research reported in this thesis is motivated by a proposal of Dr. H. Schiff for a unitary six-vector field theory. By unitary field theory we mean that matter and its properties as well as the electromagnetic field are different states of the same physical entity, a "universal field". In Dr. Schiff's view the universal field is taken to be the electromagnetic field itself, so that all matter is a manifestation of electromagnetic energy. A review of the previous attempts at such a theory, as well as some preliminary work on Dr. Schiff's theory will be found in a thesis by Teshima (1960). Since a number of Teshima's results will be used here, that work will be designated by T.

As a justification for a unitary field theory we quote the well known fact that quantum field theory is unable to predict the mass or coupling constants for the particles introduced. Neither is there any limitation to the number of kinds of particles. The hope is that these difficulties can be overcome by considering all particles as eigenstates of a universal field which is described by a universal field equation. Since only the universal field is present, all particles must arise from the interaction of this field with itself. Therefore, the basic equation must be non-linear. The universal field must also be a spinor, otherwise we could not get solutions for the fermions, i.e., from spinors (representing fermions), one can always construct tensors (representing bosons), but the converse is not true. In-

vestigations along the above lines of reasoning have been carried out by Heisenburg (1957). Heisenburg's universal field has no classical counterpart. Let us point out again that in this attempt at a unified theory of matter the electromagnetic field is considered as the universal entity. Since the electromagnetic field is a tensor, it is not reasonable to expect this theory to represent fermions. Furthermore, Dr. Schiff's theory at the present is classical; Heisenburg's is not.

Several other theoreticians, notably Chew (1961), are convinced that the Pi-Pi interaction is fundamental for all questions of strong interactions. Nevertheless, the dispersion relations do not account for the dynamics of the interaction while, in principle, a non-linear theory would be able to account for the dynamics.

We shall discuss the basic ideas of the theory only to a minimum extent, since we are primarily concerned with investigating the solutions of the static field equation in this thesis.

The fundamental equation is:

$$\left[\left(i\frac{\partial}{\partial x_\mu} - gA_\mu\right)^2 + m^2\right] F_{\rho\sigma} = 0;\ \hbar = c = 1 \tag{1-1}$$

where A_μ is a four vector potential and $F_{\rho\sigma}$ is defined by

$$F_{\rho\sigma} = \frac{\partial A_\sigma}{\partial x_\rho} - \frac{\partial A_\rho}{\partial x_\sigma} \tag{1-2}$$

as in the usual electromagnetic theory, and g is a coupling constant with the dimensions of charge. The indices run from 1 to 4, with x_1, x_2, x_3 = x, y, z; x_4 = ict; the four potential is related to the ordinary three vector potential, $\vec{A}$, and the scalar potential,

φ, by; $A_1, A_2, A_3 = A_x, A_y, A_z$; $A_4 = i\varphi$. Note that

$$\left(i \frac{\partial}{\partial x_\mu} - gA_\mu\right)^2 + m^2$$

is the Klein-Gorden operator with a self interaction.

Equation (1-1) is clearly non-linear in the four potential. Only integer spin fields can be formed from tensors and $F_{\rho\sigma}$ is a tensor with six independent components, so equation (1-1) is taken to represent bosons with integer spins including zero.

The real and imaginary parts of equation (1-1) give the two sets of equations:

$$\left[\nabla^2 - \frac{\partial^2}{\partial t^2} - m^2 - g^2(\vec{A}^2 - \varphi^2)\right] F_{\rho\sigma} = 0 \qquad (1\text{-}3)$$

$$\left[2A_\sigma \frac{\partial}{\partial x_\sigma} + \frac{\partial A_\sigma}{\partial x_\sigma}\right] F_{\mu\upsilon} = 0 \quad . \qquad (1\text{-}4)$$

(1-4) can be reduced to a simpler form by multiplying on the left by $F_{\mu\upsilon}$ and not summing over $\mu\upsilon$. This will give:

$$\frac{\partial}{\partial x_\sigma}\left[A_\sigma F^2_{\mu\upsilon}\right] = 0 \quad . \quad (\text{no sum; } \mu, \upsilon) \qquad (1\text{-}5)$$

A spin zero field is described by a scalar function so as an approximation to the spin zero case consider $\vec{A} = 0$. By using equation (1-2), the field equations will contain only the electrostatic potential, φ. If $\vec{A} = 0$, then $\vec{H} = 0$, hence the particles can have no magnetic moment. From (1-5), with $\vec{A} = 0$

$$\frac{\partial}{\partial t}\left[\varphi(\nabla\varphi)^2\right] = 0,$$

and therefore the electrostatic potential is time independent. From equation (1-3)

$$\left[\nabla^2 - m^2 + g^2\varphi^2\right] \vec{E} = 0 \quad .$$

Putting $\vec{E} = -\nabla\varphi$,

$$\nabla \left[\nabla^2 - m^2 + g^2 \frac{\varphi^2}{3} \right] \varphi = 0,$$

or, restoring $\hbar$ and c,

$$\left[\nabla^2 - \frac{m^2c^2}{\hbar^2} + \frac{g^2}{\hbar^2c^2} \; \frac{1}{3} \varphi^2 \right] \varphi = \gamma = \text{constant} \; . \qquad (1\text{-}6)$$

To get this equation in a different way, one might simply postulate a spin zero field equation of the form of a Klein-Gorden equation with a non-linear self interaction:

$$\nabla^2\varphi - \frac{1}{c^2} \frac{\partial^2\varphi}{\partial t^2} - \frac{m^2c^2}{\hbar^2} \varphi + \frac{g^2}{\hbar^2c^2} \varphi^3 = 0$$

and consider the static limit. Let us point out that the sign of the non-linear interaction is important, since a positive sign as above will lead to particle like solutions, while a negative sign will not. See N.V. Mitskevich (1956).

To get a dimensionless equation make the substitutions:

$$\varphi = \frac{g}{\lambda G} \varphi_d = \frac{mc^2}{g} \varphi_d ; \quad r = \lambda r_d$$

$$\lambda = \frac{\hbar}{mc} \; ; \quad G = \frac{g^2}{\hbar c} \; . \qquad (1\text{-}7)$$

φ_d and r_d are the dimensionless potential and radial distance, respectively. Equation (1-6) becomes:

$$\left[\nabla^2 - 1 + \frac{1}{3} \varphi_d^2 \right] \varphi_d = \frac{g\hbar^2}{m^3c^4} \gamma \; . \qquad (1\text{-}8)$$

The subscript "d" will be omitted in most of the following work. We shall only consider the special case of equation (1-8) with $\gamma = 0$. The basic equation to be studied will then be:

$$\nabla^2\varphi - \varphi + \frac{1}{3} \varphi^3 = 0 \; . \qquad (1\text{-}9)$$

If φ is to represent physical reality, φ must be continuous and

bounded everywhere.

In this work we shall investigate only those solutions with the following boundary conditions:

$$\left.\begin{array}{l} \varphi(\vec{r}) \longrightarrow 0; \quad \vec{r} \longrightarrow \infty \,, \\ \text{and for spherically symmetric solutions,} \\ \dfrac{d\varphi}{dr} = 0 \text{ at } r = 0. \end{array}\right\} \qquad (1\text{-}10)$$

Any solution of equation (1-9) satisfying these boundary conditions is called an eigensolution.

We shall now proceed to discuss the nature of these eigensolutions.

II. Phase Plane Analysis of the Radial Equation

Equation (1-9) was discussed in some detail by Finkelstein et al. (1951). We shall reproduce their analysis below.

We wish to investigate the solutions with spherical symmetry of the equation:

$$\nabla^2\varphi = \varphi - \frac{1}{3}\varphi^3 . \tag{1-9}$$

We have:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\varphi}{dr}\right) = \varphi - \frac{1}{3}\varphi^3 . \tag{2-1}$$

This equation has three trivial solutions:

$$\varphi = \text{constant} = K$$

with

$$K = 0; \quad K = \pm\sqrt{3} . \tag{2-2}$$

Let us find the behaviour of the solutions near these special points. To do this set

$$\varphi = K + U(r) \tag{2-3}$$

and regard $U(r)$ small with respect to K. We can neglect the non-linear term obtained by substituting (2-3) into (2-1). We get:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dU}{dr}\right) \simeq U(r) \qquad \text{near } K = 0, \tag{2-4A}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dU}{dr}\right) \simeq \pm\sqrt{3} + U(r) - \frac{1}{3}(\pm 3\sqrt{3} + 9U(r)) \tag{2-4B}$$

$$\simeq -2U(r) \qquad \text{near } K_{\pm} = \pm\sqrt{3} .$$

In general the solution of

$$\frac{1}{r^2}\frac{d}{dr}(r^2 \frac{dU}{dr}) = - kU$$

may be found by letting $U = \frac{f}{r}$, then $\frac{d^2f}{dr^2} = - kf$

hence

$$f = Ur = A \sin(\sqrt{k} + \alpha) \qquad \text{for } k > 0$$

$$f = Ur = A e^{-\sqrt{k}\, r} \qquad \text{for } k < 0$$

Then we see that:

Near $K_{\pm} = \pm \sqrt{3}$ where $k = + 2$
the solution is trigonometric. (2-5A)

Near $K = 0$ where $k = - 1$
the solution is exponential. (2-5B)

To investigate the solutions further let us now make a plot of what is happening in the phase plane. Let φ and $\varphi' = \frac{d\varphi}{dr}$ correspond to the "position" and "velocity" of a point in phase space. We are now thinking of the position r as "time" to obtain an analogy with the dynamical case. Then equation (2-1) corresponds to a non-conservative one dimensional motion, since r (the time) appears explicity. Rewriting equation (2-1):

$$\varphi'' + \frac{1}{3}\varphi^3 - \varphi = - \frac{2}{r}\frac{d\varphi}{dr} \qquad (2\text{-}6)$$

or:

$$\frac{d}{dr}\left[\frac{1}{2}(\varphi')^2 + \frac{1}{12}\varphi^4 - \frac{1}{2}\varphi^2\right] = - \frac{2}{r}(\frac{d\varphi}{dr})^2 \qquad (2\text{-}7)$$

When the motion is conservative the particle (of mass = 1) satisfies equations (2-6) and (2-7) with the right hand side set equal to zero. From equation (2-7) we see that the energy, E, for the conservative motion is:

$$E = \frac{1}{2}(\varphi')^2 + V(r)$$

where $$V(r) = \frac{1}{12}\varphi^4 - \frac{1}{2}\varphi^2$$

$V(r)$ is the potential energy. The equilibrium points of the motion are given by $\frac{\partial V}{\partial \varphi} = 0$ and correspond to the special solutions $\varphi = 0, \pm\sqrt{3}$. A point representative of the conservative motion moves along the lines of constant E in the phase plane. For given E we can now make a plot of the conservative motion in the phase plane. This is shown in Figure 1. The curve for $E = 0$ is a figure eight through the origin; the curves $E > 0$ enclose both $K_\pm$ and $K = 0$, but the curves $E < 0$ enclose only one of the solutions K_+ or K_-.

The non-conservative motion, which corresponds to our actual problem may now be described. From equation (2-7) we see that $\frac{dE}{dr} = -\frac{2}{r}(\frac{d\varphi}{dr})^2$. This term represents the dissipation of energy with time. Therefore, since $\frac{dE}{dr}$ is never positive the representative point of the actual motion must always move inward across the lines of constant E. Such a line must always end at either $K_\pm$ or the origin, no matter where it starts. In particular, if any solution curve gets into the shaded region, it must terminate on either K_+ or K_-.

The solution curve labled eo is designated as an "eigensolution". These solutions are finite at the origin and approach zero as $r \longrightarrow \infty$. This follows from equation (2-5B). An eigensolution is located by starting on the φ axis and continuously increasing the initial value, $\varphi(0)$. At first when $0 < \varphi(0) < \sqrt{6}$

Figure 1

A sketch of the phase plane for depicting solutions of radial symmetry. The curves beginning at k_+ and k_- are solutions asymptotic to $\pm\sqrt{3}$ while the curve eo is an "eigensolution".

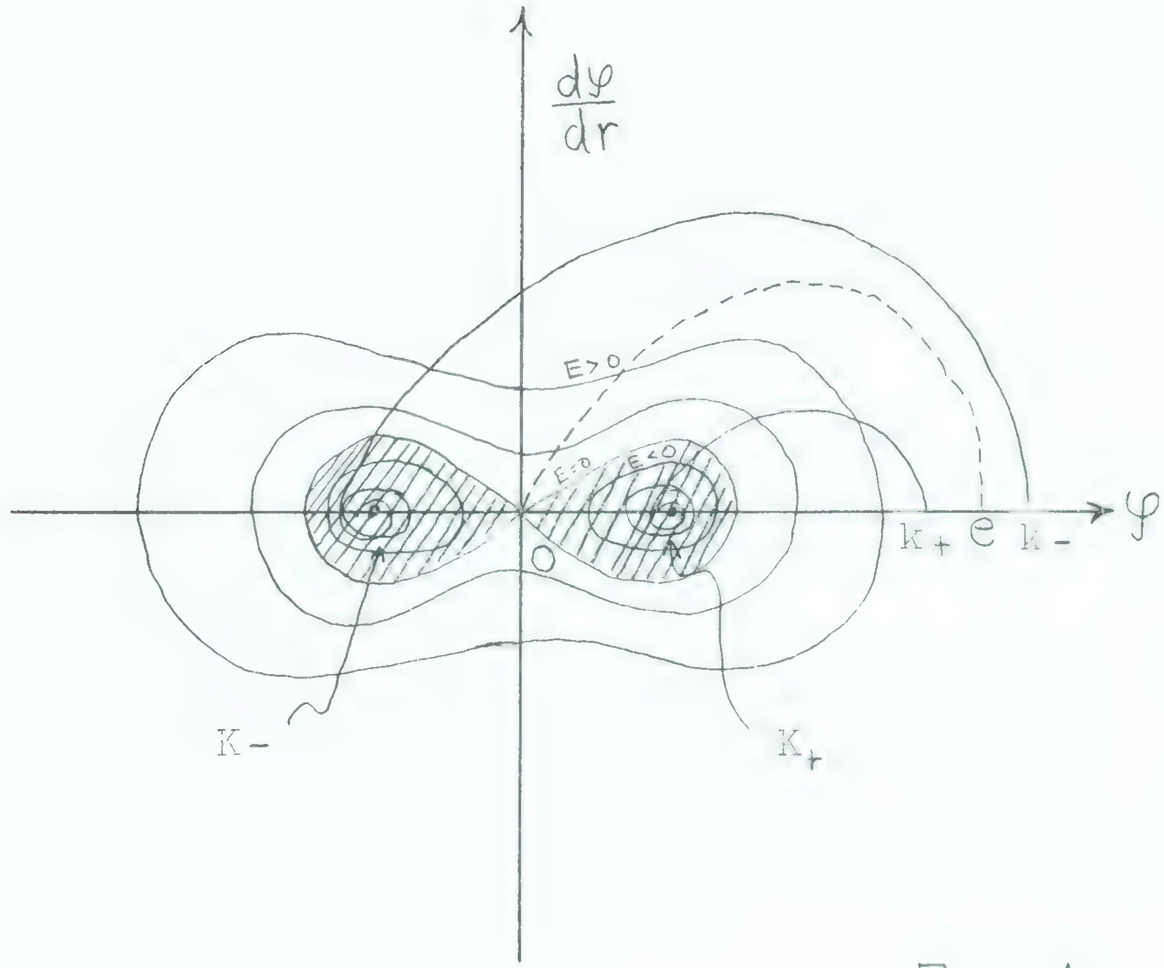


Fig. 1.

all solutions are certain to terminate on K_+. The situation is still the same for $\varphi(0) = k_+$ which is larger than the critical value, $\sqrt{6}$. But for a value $\varphi(0) = k_-$ the solution will terminate on K_-. For some value $\varphi(0) = e$ between k_+ and k_- the solution will terminate at the origin. By narrowing the interval $k_+ \, k_-$ the eigensolution may be determined with arbitrary accuracy.

The above analysis yields the following facts concerning the solutions of the equation $\nabla^2\varphi = \varphi - \frac{1}{3}\varphi^3$ for radial symmetry.

1. Every solution must behave at infinity either as

a) $\varphi \longrightarrow \dfrac{\sin(\sqrt{2}\, r + \alpha)}{r} \pm \sqrt{3}$

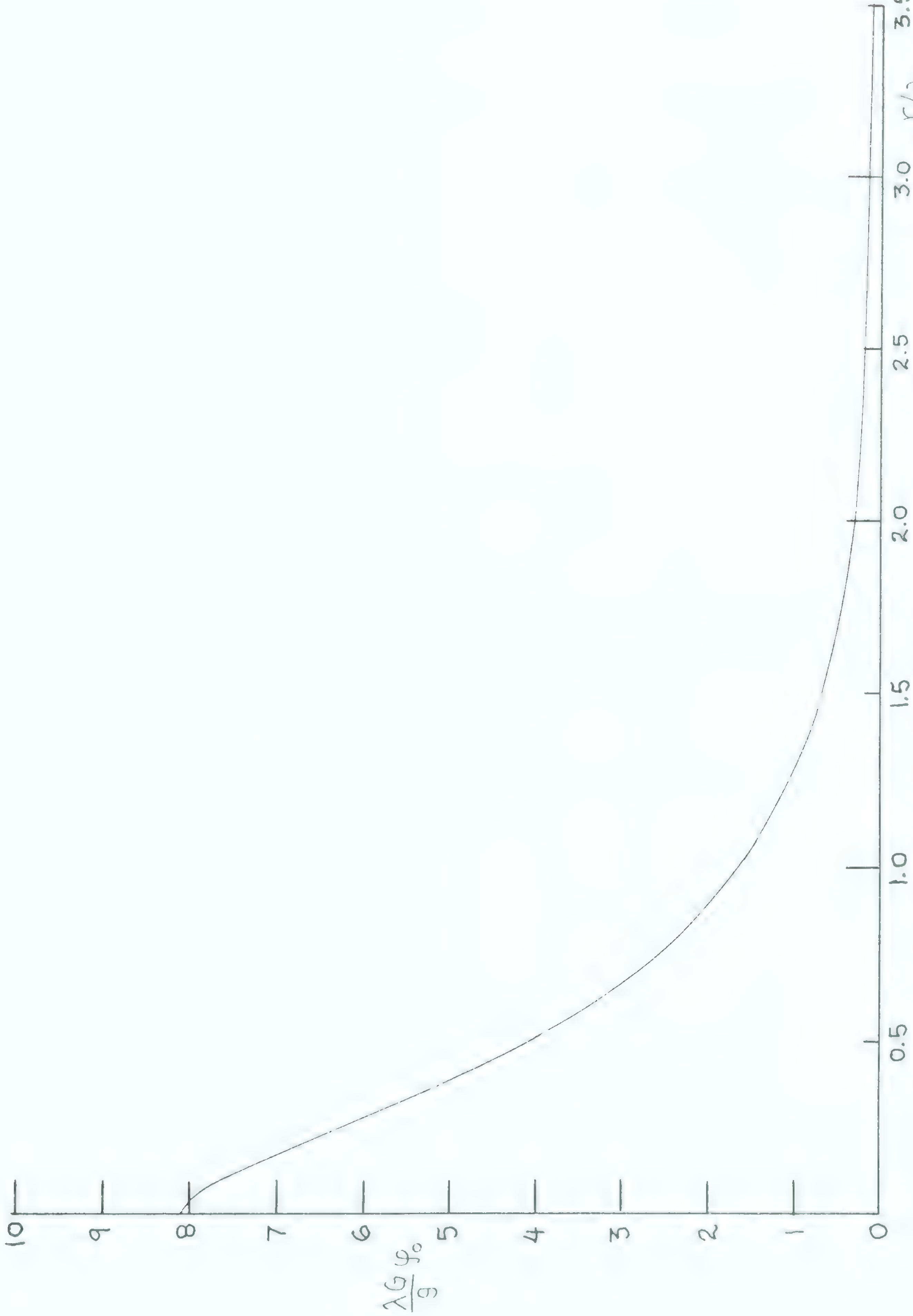
or b) $\varphi \longrightarrow \dfrac{e^{-r}}{r}$

2. No solutions exist for which $\varphi'(0) = 0$ and $\varphi(0) = 0$ except the trivial one $\varphi = 0$.
3. No eigensolution's solutions exist for $\varphi'(0)$ and $\varphi(0) < \sqrt{6}+$
4. If we require that φ' be zero at the origin, then the solutions of the type a) form a continuous set, while those of type b) form a discrete set.
5. The solutions forming the discrete set have zero, one, two, etc., nodes corresponding to the solution being the first, second, third, etc., eigensolution.

The first three solutions of the type b) were computed by numerical integration of equation (2-1); the detailed discussion will be found in T. The solutions with no node, one node, and two nodes are designated by φ_o, φ_1 and φ_2 respectively, and the first two are reproduced here in Figures 2 and 3.

Figure 2

The first eigensolution, φ_0, of spherical symmetry obtained by numerical integration of equation (1-9). Reproduced from Teshima, (1960).



10
9
8
7
6
5
4
3
2
1
0
$\frac{\lambda G}{g} \varphi_0$
0.5
1.0
1.5
2.0
2.5
3.0
3.5
r/λ

Fig. 2.

Figure 3

The second eigensolution, φ_1, of spherical symmetry obtained by numerical integration of equation (1-9). Reproduced from Teshima, (1960).

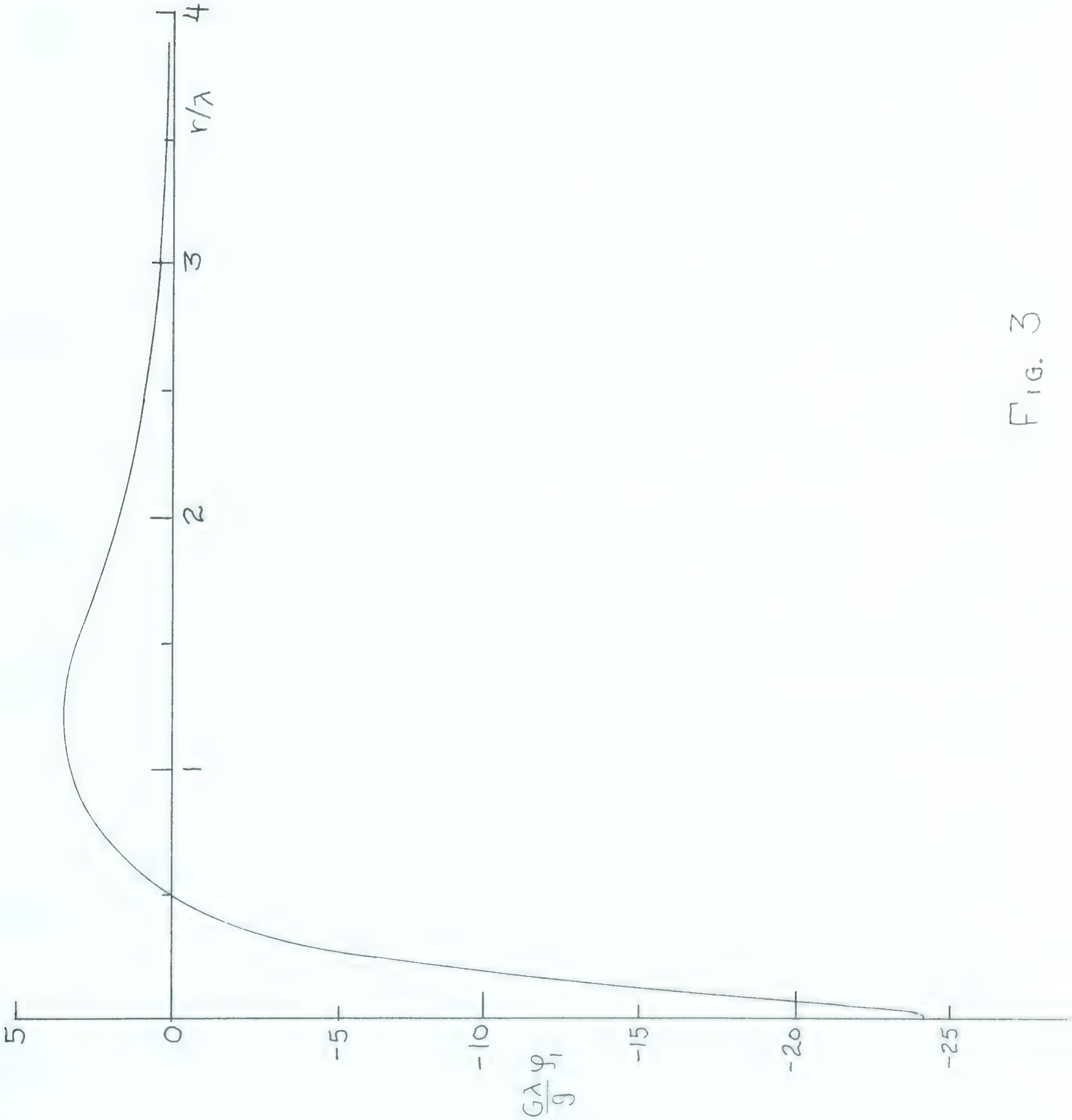


FIG. 3

III. Bound States

If the discrete solutions of equation (1-1) represent particles, it is important to compute the interaction between solutions, i.e., particles of different kinds. Note that this interaction would be purely electromagnetic and in the static approximation could be represented by an interaction potential energy curve. The difficulty in finding a proper expression for the energy of the field has been stressed in T. Since a Lagrangian for the theory has not been found, an "ad hoc" expression for the energy and the interaction energy of the field must be used.

We assume for the energy the expression

$$E = \int \rho\varphi dv \tag{3-1}$$

where ρ is the charge density, and satisfies

$$-4\pi\rho = \nabla^2\varphi \quad . \tag{3-2}$$

Upon converting the ρ and φ to dimensionless quantities, using equations (1-7)

$$E = \frac{mc^2}{G} \int \rho_d \varphi_d dv$$

is obtained; all of our energies will be in units of $\frac{mc^2}{G}$.

Extending (3-1) to two particles, we define the total energy as

$$E_T = \int (\rho_1 + \rho_2)(\varphi_1 + \varphi_2) dv \quad . \tag{3-3}$$

When the systems are far apart we know that

$$E_T = \int \rho_1\varphi_1 dv + \int \rho_2\varphi_2 dv \quad . \tag{3-4}$$

Hence the interaction energy, E_I, is given by the difference be-

tween (3-3) and (3-4), namely

$$E_I = \int \rho_1 \varphi_2 dv + \int \rho_2 \varphi_1 dv$$

$$= 2 \int \rho_1 \varphi_2 dv = \quad 2 \int \rho_2 \varphi_1 dv$$

(It was shown in T. that $\int \rho_1 \varphi_2 dv = \int \rho_2 \varphi_1 dv$.) For an arbitrary separation, $\vec{d}$, of the systems one and two, the interaction energy, written in full is:

$$E_I(\vec{d}) = 2 \int \rho_1(\vec{r}\,')\varphi_2(\vec{d} - \vec{r}\,')\overrightarrow{dr'}$$

or (3-5)

$$= 2 \int \rho_1(\vec{r} - \vec{d})\varphi_2(\vec{r})\overrightarrow{dr}, \text{ etc.}$$

(Note that Teshima's expression for the interaction energy differs from ours by the factor of two.)

The possibility of forming bound states between particles of the type φ_0 and φ_1 has been discussed in T. The interaction energy, V_{01}, for an arbitrary separation of these particles is plotted in Figure 4. This energy curve was obtained by fitting analytic functions to the numerical solutions of φ_0 and φ_1 and calculating the integral (3-5). An attempt was made in our work to compute the interaction by direct numerical integration using the numerical solutions φ_0 and φ_1. We had hoped to gain additional accuracy over Teshima's potential by eliminating the need to "fit" the numerical solutions with functions. The attempt failed, evidently because the numerical solutions were not computed for enough points, this caused the potential to undergo wild variations.

If the bound state is formed classically, it is readily seen from Figure 4 that the binding energy, B , will be 12.84 $\frac{mc^2}{G}$

Figure 4

The black curve shows the interaction potential energy, V_{01}, between particles of the first and second kinds. Reproduced from Teshima, (1960). The square well approximation is shown by the dotted curve.

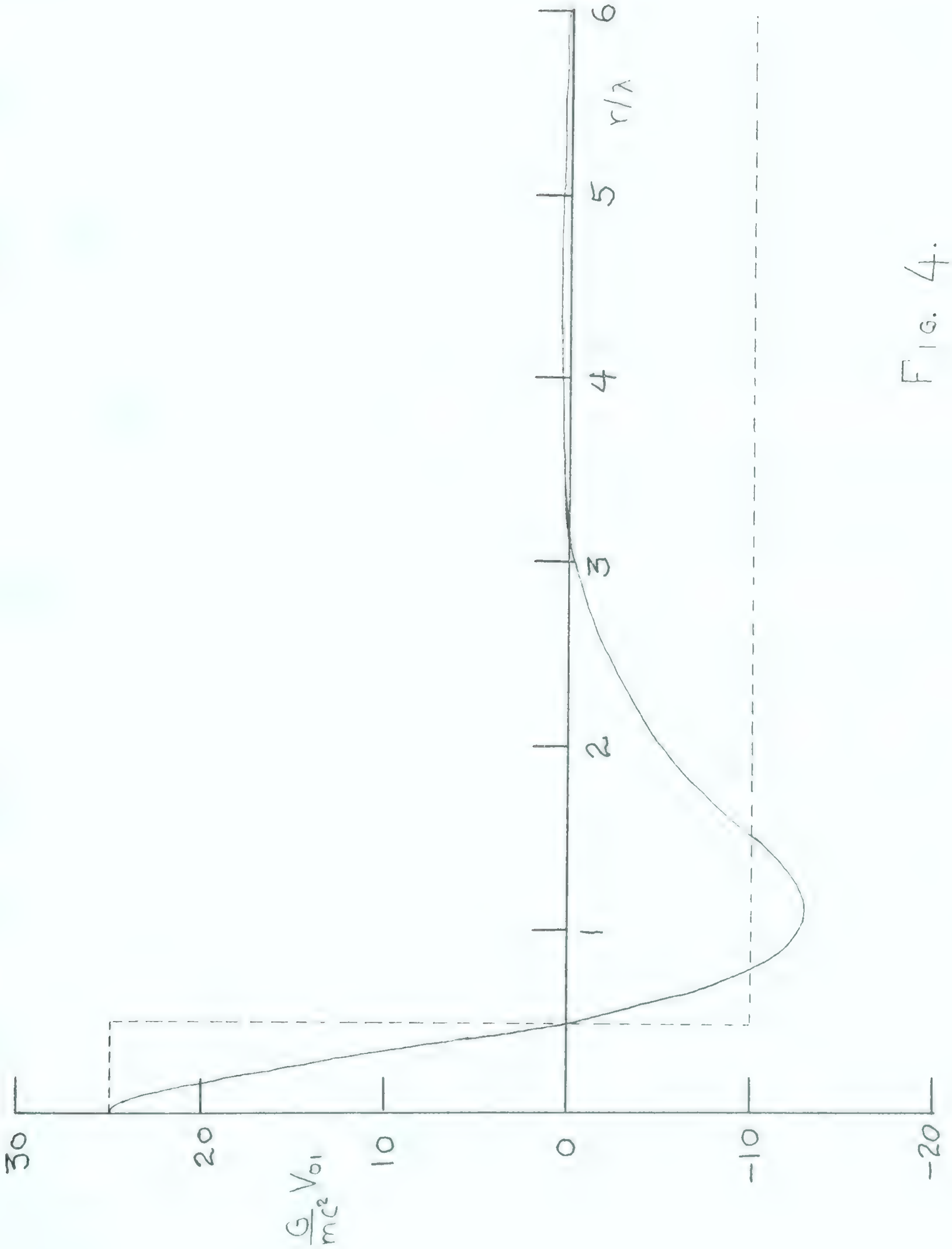


Fig. 4.

with a separation, r, of 1.0λ.

To solve the quantum mechanical problem for the binding energy a tractable form for the potential, V_{01}, is needed. The Morse potential

$$V = V_o \left[e^{-2(r-r_o)/a_o} - 2e^{-(r-r_o)/a_o} \right] \tag{3-6}$$

has been plotted on Figure 5 together with V_{01}. The figure shows that this function is a good approximation to V_{01}, at least in the region of the well, where it is most important to have a good fit. Any further improvement in trying to fit an analytical curve to V_{01} is unwarranted, since the existing V_{01} has been obtained by an approximation.

The energy, B_n, of the bound states for the potential (3-6) is found in Morse and Feshbach, Methods of Theoretical Physics (1953).

$$B_n = -V_o + \frac{\hbar}{a_o}\sqrt{\frac{2V_o}{m}}\left(n+\frac{1}{2}\right) - \frac{\hbar^2}{2ma_o^2}\left(n+\frac{1}{2}\right)^2$$

for L = 0 and $e^{r_o/a_o} \gg 1$. n is any integer $< \frac{a_o}{\hbar}\sqrt{2mV_o} - \frac{1}{2}$. Converting these to the dimensionless form by using the relations (1-7):

$$B_n = mc^2\left[\frac{-V_o}{G} + \frac{2}{a_o}\sqrt{\frac{V_o}{2G}}\left(n+\frac{1}{2}\right) - \frac{1}{2a_o^2}\left(n+\frac{1}{2}\right)^2\right]$$

and (3-7)

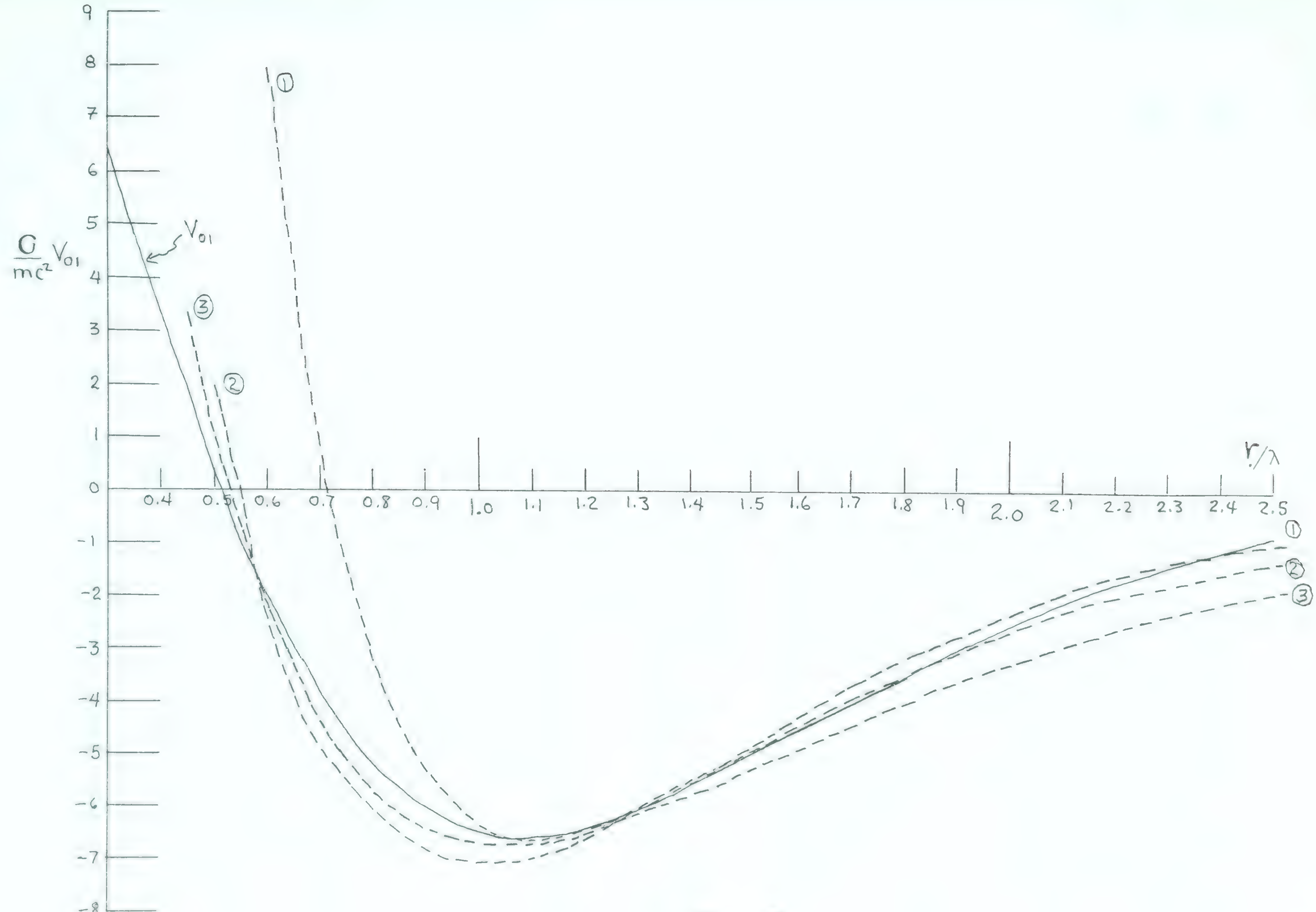
$$n < 2a_o\sqrt{\frac{V_o}{2G}} - \frac{1}{2}$$

Following Teshima the energy of the 1st and 2nd particles is taken to be: (pages 53, 54 of T.)

$$E_0 = \frac{mc^2}{G}\,(13.53); \quad E_1 = 6.293\,E_0 \tag{3-8}$$

Figure 5

The solid curve shows the interaction potential energy, V_{01}, while the dashed curves are the Morse potential approximations. The parameters for the Morse potential curves are given in Appendix D.



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0
-1
-2
-3
-4
-5
-6
-7
-8
$\frac{G}{mc^2}V_{01}$
V_{01}
r/λ
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2.0
2.1
2.2
2.3
2.4
2.5
1
2
3

Fig. 5.

The number 13.53 and the ratio E_0/E_1 is not arbitrary since they are a direct result of the non-linearity of the field equations together with the fact that we are getting something similar to eigensolutions of a linear equation for the solutions φ_0 and φ_1. If the energy of the basic or first particle is to be equal to mc^2, we must take the coupling constant to be

$$G = 13.53 \ . \tag{3-9}$$

Inserting numerical values, we find that for the three Morse potential curves plotted in Figure 5, n is any integer less than about 1/2. Therefore, n = 0, and there is only one bound state.

Using (3-7), (3-8) and (3-9) the total energy, E_T, of the bound system of particles φ_0 and φ_1 can be calculated using:

$$E_T = E_0 + E_1 - B_1 \tag{3-10}$$

A table of values of B_n and E_T is shown below for the three Morse potential curves plotted on Figure 5.

Table 1

Quantum Mechanical bound states between

φ_0 and φ_1

Curve	1	2	3
B_0	0.119	0.231	0.250
E_T	7.174	7.062	7.043

Energies are in units of mc^2 with G = 13.53 .

This does not exhaust the possibility of forming bound states between the solutions φ_0 and φ_1. As can easily be seen, if φ is a solution to equation (1-9), then $-\varphi$ is also a

solution. Therefore, besides the potential V_{01} which is essentially repulsive near the origin, $- V_{01}$ is also a possible potential curve which is attractive near the origin. As an estimate of the quantum mechanical bound states with this attractive potential, $- V_{01}$ was approximated by a square well potential:

$$\left.\begin{array}{ll} V_{01} = -30 & 0 < r < 0.5 \\ V_{01} = 0 & r > 0.5 \end{array}\right\} \text{dimensionless units}$$

The minimum well depth for forming one bound state in a potential well of depth, V, and width, a, is given by:

$$Va^2 > \frac{\pi^2 \hbar^2}{8} \quad .$$

Converting to dimensionless units:

$$V_d a_d^2 > \frac{\pi^2 G}{8}$$

Inserting numbers, the left hand side gives 8.74 while the right is 16.7. $V_d a_d^2$ is too small by a factor of 2, which is significant even with the crude square well approximation, to give a quantum mechanical bound state.

The total energy of the classically bound particle in this potential is found to be $E_T = 5.47\ mc^2$, with a binding energy, $B = 1.82\ mc^2$.

Teshima also has calculated the potential energy curve for the interaction of two particles of the first kind, i.e., φ_o and φ_o. This energy curve is called V_{00} and is reproduced from T. and shown in Figure 6. This potential is essentially repulsive near the origin, but if the sign of one of the solu-

Figure 6

The interaction potential energy between two solutions of the first kind is given by the solid curve. Reproduced from Teshima, (1960). The dashed curve is the exponential approximation.

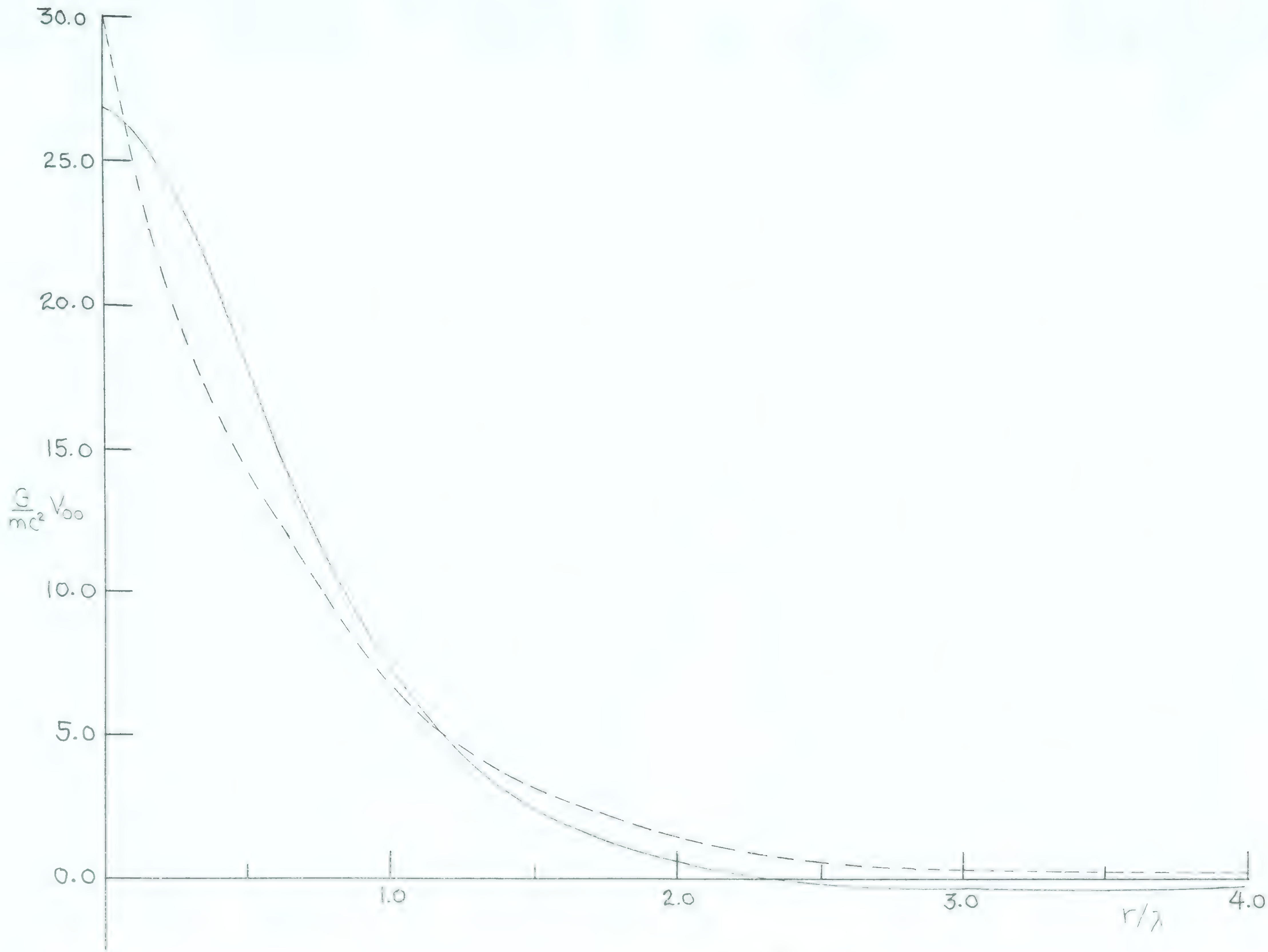

Fig. 6.

tions φ_0 is changed, the potential will be attractive. To investigate the possibility of forming a quantum mechanical bound state for this situation, $-V_{00}$ was approximated with the function

$$V = -B_d\, e^{-r_a/a_d}.$$

If

$$B_d \approx 30;\; a_d \approx \frac{1}{1.5}$$

then V approximates $-V_{00}$ quite well as is shown in Figure 6. The analysis of the Schrodinger equation for a potential of the form, $V = B\, e^{-r/a}$, shows that no bound state will be formed unless the condition

$$2a\sqrt{\frac{2\mu B}{\hbar^2}} \geqslant 2.405$$

holds. The constant 2.405 is the first zero of the zero'th order bessel function of the first kind, and μ is the reduced mass. Using the dimensionless units together with the fact that the masses of the two systems $-\varphi_0$ and φ_0 are equal, the condition is:

$$B_d a_d^2 \geqslant \left(\frac{2.405}{2}\right)^2 G$$

The numerical values for a_d, B_d, and G give 13.3 for the left hand side and 19.5 for the right. Again the well is probably not deep enough to have a bound state.

The binding energy for the classically bound particle is equal to the energy of the two separate parts and therefore the total energy is zero.

The potential energy curves V_{00} and V_{01} still show the

possibility of forming several other classical bound states. These states occur in both cases for a separation of the particles of the order of 4λ and have a very small binding energy. Since the potential curves used are only approximations, the existance of these bound states is doubtful and are listed only for completeness. A more accurate investigation of the interaction potentials will have to be made to determine if these states exist.

A summary of the results obtained above is shown in Tables 2 and 3. Further discussion of the physical interpretation of these bound states will be found in Chapter 6 of this work.

Table 2

Summary of Bound States

Interaction	Quantum Mechanical Bound States	Classical Bound States
$\varphi_0(+\varphi_0)$	none (repulsive)	none
$\varphi_0(-\varphi_0)$	none or possibly $B \approx 0$; $E = 2$	none
$\varphi_0(+\varphi_1)$	one $B \approx 0.19$; $E \approx 7.10$	one $\vec{r} = 1.0\lambda$ $B = 0.946$; $E = 6.35$
$\varphi_0(-\varphi_1)$	none	one $\vec{r} = 0$ $B = 1.83$; $E = 5.47$

Table 3

Doubtful Bound States

Interaction	Quantum Mechanical Bound States	Classical Bound States
$\varphi_0(+\varphi_0)$	none	$\vec{r} \approx 3\lambda$ $B \approx 0.206;\quad E \approx 2$
$\varphi_0(-\varphi_1)$	none	$\vec{r} \approx 4\lambda$ $B \approx 0.486;\quad E \approx 7.29$

B = binding energy of system of particles composed of particles $\varphi_i(\pm\varphi_j)$

E = total energy of the system

$\vec{r}$ = classical separation of the particles

B and E are in units of mc^2 with the coupling constant $G = 13.53$

IV. The Variational Method (V.M.)

It is well known that the solution to a linear differential equation is the extremum of a certain integral, usually called the Lagrangian, where several subsidiary or auxiliary conditions may be required. In general the differential equation is the Euler equation for the Lagrangian.

It is easily seen that equation (1-9) is the Euler equation for the Lagrangian,

$$L = \frac{3}{8\pi}\int\left[\varphi^2 + (\nabla\varphi)^2 - \frac{1}{6}\,\varphi^4\right] dv \quad . \tag{4-1}$$

The integral is taken over all space and φ must satisfy either $\varphi \longrightarrow 0$ as $r \longrightarrow \infty$, or $\frac{d\varphi}{dn} \longrightarrow 0$ as $r \longrightarrow \infty$. $\frac{d\varphi}{dn}$ is the normal derivative of φ on a surface. Thus, the solutions of equation (1-9) satisfying the boundary condition (1-10) are the extremals of the above Lagrangian.

It will be shown later that the constant, $\frac{3}{8\pi}$, in (4-1) is chosen so that L will be equal to what has been defined as the energy of the field.

The difficulty with the above variational method is that the second order variational terms are not positive or negative definite, so one has no assurance that the method provides an upper or lower bound to L. This is shown in Appendix B.

In order to remove the above difficulty concerning the bounds of L, it is necessary to reformulate the variational principle in a different way. Before doing this, it is necessary to

know that the solutions of equation (1-9) satisfy the following integral relationship:

$$3\int\left[\varphi^2 + (\nabla\varphi)^2\right]dv = \int\varphi^4 dv .$$

This equation together with the following three integral relationships are proved in Appendix A.

$$3\int\varphi dv = \int\varphi^3 dv \qquad (4\text{-}4)$$

$$12\int\varphi^2 dv = \int\varphi^4 dv \qquad (4\text{-}5)$$

$$3\int\varphi^2 dv = \int(\nabla\varphi)^2 dv \qquad (4\text{-}6)$$

As a consequence of the last two relationships, note that the energy of the field φ, interacting with itself, as calculated from the definitions (3-1) and (3-2) is

$$E = -\frac{1}{4\pi}\int\varphi\nabla^2\varphi dv .$$

Then by Green's theorem,

$$E = \frac{1}{4\pi}\int(\nabla\varphi)^2 dv . \qquad (4\text{-}7)$$

The same expression is obtained by using the integral relationships (4-5) and (4-6) in the Lagrangian (4-1). Thus for an extremal, the Lagrangian is positive definite and is equal to the energy of the field.

To reformulate the variational problem so that the eigensolutions always make the Lagrangian a minimum we must consider either of the two problems:

I. Extremize $L = \frac{3}{4\pi} \int \varphi^2 dv$ (4-8)

subject to the auxiliary conditions,

$$J = 12 \int \varphi^2 dv - \int \varphi^4 dv = 0 \tag{4-9}$$

and

$$K = 3 \int \varphi^2 dv - \int (\nabla\varphi)^2 dv = 0 \, . \tag{4-10}$$

II. Extremize $L = \frac{3}{16\pi} \int \left[\varphi^2 + (\nabla\varphi)^2\right] dv$ (4-11)

subject to

$$M = 3 \int \left[\varphi^2 + (\nabla\varphi)^2\right] dv - \int \varphi^4 dv = 0 \, . \tag{4-12}$$

To show that the extremals of the above variation problems satisfy equation (1-9) use the method of undetermined Lagrange multipliers.

I'. Extremize $L' = L + \lambda J + \mu K$ (4-13)

where λ and μ are the Lagrange multipliers to be determined. The Euler equation becomes

$$\mu\nabla^2\varphi + (3 + 12\lambda + 3\mu)\varphi - 2\lambda\varphi^3 = 0 \, . \tag{4-14}$$

Multiply (4-14) by φ, integrate, use Green's theorem and the auxiliary conditions (4-9) and (4-10) to get $\lambda = 1/4$ and the Euler equation is:

$$\mu\nabla^2\varphi + (6 + 3\mu)\varphi - \frac{1}{2}\varphi^3 = 0 \, . \tag{4-15}$$

In the same way that the integral relation (4-5) was shown to hold for solutions of equation (1-9), it can be shown that the

solutions of (4-15) satisfy

$$\int \varphi^4 dv = 8(6 + 3\mu) \int \varphi^2 dv \quad . \tag{4-16}$$

But (4-16) is required simultaneously with (4-9), therefore $\mu = -3/2$ and the Euler equation is identical to equation (1-9).

The second problem is easier.

II'. Extremize $L' = L + \lambda M$ (4-17)

where λ is the Lagrange multiplier. The Euler equation is:

$$(\tfrac{3}{4} + 3\lambda)(\varphi - \nabla^2\varphi) - 2\lambda\varphi^3 = 0 \quad . \tag{4-18}$$

Multiply (4-18) by φ, integrate, use Green's theorem and the auxiliary condition (4-12) to obtain $\lambda = 1/4$. The Euler equation (4-18) is identical to equation (1-9) with this value of λ.

To see that the extremals which approach zero at infinity make the Lagrangian in the above problems a minimum, note that in both cases the Lagrangian (L) is a positive definite quantity. If the auxiliary conditions are not imposed, the second order variational terms of L are positive definite. This can be seen by an analysis analogous to that given for the Lagrangian (4-1) in Appendix B. Now, if any number of auxiliary conditions are imposed, they can only serve to raise the value of the minimum. See page 407, Courant and Hilbert, Methods of Mathematical Physics, Vol. 1.

In all of the above problems, the extremal which makes

L an absolute minimum is $\varphi = 0$.

To obtain the remaining solutions it is necessary to develop a variational method for "excited" states. To do this a connection is needed between the two solutions, φ_1 and φ_2, of equation (1-9). This connection is furnished by the so called orthogonality relation,

$$\int \varphi_1 \varphi_2^3 \, dv = \int \varphi_1^3 \varphi_2 \, dv \ , \tag{4-19}$$

which is proved in Appendix A.

Now consider the variational problem:

III. Extremize $L = \frac{3}{16\pi} \int \left[\varphi_2^2 + (\nabla\varphi_2)^2 \right] dv$ (4-20)

subject to

$$M = 3 \int \left[\varphi_2^2 + (\nabla\varphi_2)^2 \right] dv - \int \varphi_2^4 \, dv = 0 \tag{4-12}$$

and

$$N = \int \left[\varphi_1^3 \varphi_2 - \varphi_2^3 \varphi_1 \right] dv = 0 \ , \tag{4-21}$$

where φ_1 is known and satisfies $\nabla^2\varphi_1 = \varphi_1 - \frac{1}{3} \varphi_1^3$.

Whether or not we regard $\varphi_1 = 0$ as the first solution makes no material difference as the condition (4-21) is satisfied identically and problem III then reduces to problem II. Thus, the first non-zero solution of equation (1-9) is given by that extremal of problem II which now gives the lowest value for the Lagrangian not equal to zero.

To obtain further solutions, consider variational pro-

blem III again, but with the requirement that φ_1 be equal to the non-zero solution found above. This time the orthogonality relation will be important, since it is not identically satisfied.

To determine the Euler equation consider:

III'. Extremize $L' = L + \lambda M + \mu N$ (4-22)

where λ and μ are the Lagrange multipliers. The function φ_1 is known and satisfies $\nabla^2\varphi_1 = \varphi_1 - \frac{1}{3}\varphi_1^3$. The Euler equation is

$$(\tfrac{3}{4} + 3\lambda)(\varphi_2 - \nabla^2\varphi_2) - 2\lambda\varphi_2^3 + \tfrac{\mu}{2}(3\varphi_2^2\varphi_1 - \varphi_1^3) = 0 \ . \qquad (4\text{-}23)$$

To determine the constant μ, note that under the transformation $\varphi_2 \longrightarrow -\varphi_2$, L and M remain invariant. Further, N is also invariant since it is equal to zero. Therefore the Euler equation satisfied by $-\varphi_2$ must be identical to the equation satisfied by φ_2. But from (4-23) with φ_2 replaced by $-\varphi_2$ there results,

$$-(\tfrac{3}{4} + 3\lambda)(\varphi_2 - \nabla^2\varphi_2) + 2\lambda\varphi_2^3 + \tfrac{\mu}{2}(3\varphi_2^2\varphi_1 - \varphi_1^3) = 0 \ . \qquad (4\text{-}24)$$

Adding (4-24) and (4-23) we have

$$\mu(3\varphi_2^2 - \varphi_1^2)\varphi_1 = 0 \ .$$

Therefore $\mu = 0$, since $\varphi_1 \neq 0$ and $\varphi_1^2 \neq 3\varphi_2^2$.

To obtain the value for λ proceed as in problem II'. Again $\lambda = 1/4$ and the Euler equation is identical to equation (1-9).

Thus formulated, it is seen that the above variational problems can be used to find approximate solutions of equation (1-9). It is only necessary to chose trial functions which satisfy the required auxiliary conditions for the Lagrangian to assume a value at its minimum which is higher than the actual value. In the remaining part of this work several examples will be presented, but it should be pointed out that the above variational problems have not been applied systematically, since most of the variational theory was formulated after working out the results of many trial functions.

To be more specific let us now describe the content of the variational method (V.M.). This method attempts to approximate the solutions of equation (1-9) by substituting a trial function, $\varphi_T(\alpha_1, \alpha_2 \ldots \alpha_n; \vec{r})$, which must satisfy certain auxiliary conditions, into a Lagrangian. The Lagrangian is then minimized or maximized with respect to the parameters of the trial function. Let these parameters be α_i, then

$$L_T(\alpha_i) = L(\varphi_T) \; .$$

The condition that the integral be made an extremum leads to the simultaneous equations,

$$\frac{\partial L_T}{\partial \alpha_i} = 0 \; ; \quad (i = 1,2,\ldots.n) \; . \qquad (4\text{-}26)$$

The solution of these n equations determine the optimum values of α_i and therefore the best possible trial function of the form used. The particular form used initially for the trial function

is suggested by some a priori guesses as to the nature of the exact solution.

The V.M. is a powerful tool with which we can approximate the solutions of a non-linear differential equation which cannot be solved. One great advantage of the V.M. is that we now have a method to attack the solutions of equation (1-9) which are not spherically symmetric. One must, of course, show that the solutions of more complicated symmetry exist, but this problem has generally been ignored in this work.

V. Calculations Using the V.M.

In this section we shall present the results of the analysis using the V.M. for several types of solutions to equation (1-9). Before presenting the results for the specific functions we shall discuss two points of general interest.

1. Green's function method of improving the trial functions.

A method of improving the trial functions can be devised by writing equation (1-9) in the form

$$\nabla^2\varphi - \varphi = 4\pi\rho(\vec{r}) \tag{1-9a}$$

where

$$\rho(\vec{r}) = -\frac{1}{12\pi}\varphi^3(\vec{r}) \ . \tag{1-9b}$$

The solution of equation (1-9a) is given by

$$\varphi_G(\vec{r}) = \int G(\vec{r},\vec{r}\,')\rho(\vec{r}\,')d\vec{r}\,' \tag{5-1}$$

where $G(\vec{r},\vec{r}\,')$ is the Green's function for the operator $(\nabla^2 - 1)$ and $\rho(\vec{r})$ is assumed known. Now let

$$\rho(\vec{r}) = -\frac{1}{12\pi}\varphi_T^3\,(\vec{r};\ \alpha_1\ldots.\alpha_n), \tag{5-2}$$

then $\varphi_G(\vec{r};\ \alpha_1\ldots.\alpha_n)$ should be a better approximation to the eigensolution of equation (1-9). It was shown in T. that φ_G indeed is a better approximation for the nodless spherically symmetric solutions. Note, however, that we do not have any general proof that after n such operations implied by (5-1), φ_G will approach the actual solution. In any case, if φ_G contains some parameters, they can now be determined by the V.M. Another procedure is to

determine the parameters in φ_T first by the V.M., insert the numerical values, then find φ_G from equation (5-1). The difference between the energies obtained by these two methods is small if the trial functions are spherically symmetric.

2. Auxiliary conditions and a specialized form of the Lagrangian (4-1).

Besides the extremization conditions on the Lagrangian of a trial function, one or more integral relationships as well as possible orthogonalization conditions must be satisfied by the trial function. Therefore, for any trial function, φ_T, there are three kinds of equations which may be required.

n Extremization conditions

$$\frac{\partial I_T}{\partial \alpha_i} = 0 \qquad (i = 1,2\ldots.n) \tag{5-3}$$

Three possible integral relationships

$$12\int \varphi_T^2 \, dv = \int \varphi_T^4 \, dv \tag{5-4}$$

$$3\int \varphi_T^2 \, dv = \int (\nabla\varphi_T)^2 dv \tag{5-5}$$

$$3\int \varphi_T \, dv = \int \varphi_T^3 \, dv \tag{5-6}$$

Orthogonality conditions

$$\int \varphi_T^3 \, \varphi_i dv = \int \varphi_T \, \varphi_i^3 dv \qquad (i = 1,2\ldots.k) \tag{5-7}$$

Note that any of the auxiliary conditions used in the variational problems of the preceeding chapter may be formed from these

integral conditions.

One of the extremization equations (5-3) is always equivalent to the integral relation (4-12). This can be quickly verified by letting $\varphi_T = A\eta(\vec{r})$, where A is a constant, in the Lagrangian (4-1). The equation $\frac{\partial L}{\partial A} = 0$ yields the desired relation (4-12). Therefore the results of method II or III will apply if the above extremization has been used, even though the Lagrangian (4-1) is minimized.

A large number of the three parameter trial functions investigated reduce the Lagrangian (4-1) to a similar form. In this case, two of the extremization conditions (5-3) are equivalent to the two integral relations (5-4) and (5-5). To be more specific, the specialized form of the Lagrangian (4-1) will be obtained if the integrals in the Lagrangian reduce to: (The integrals (5-11) and (5-12) are included for future reference.)

$$\frac{1}{4\pi}\int \varphi_T^2 \, dv = \frac{B^2}{\beta^3} Q_1(p) \tag{5-8}$$

$$\frac{1}{4\pi}\int \varphi_T^4 \, dv = \frac{B^4}{\beta^3} Q_3(p) \tag{5-9}$$

$$\frac{1}{4\pi}\int (\nabla\varphi_T)^2 dv = \frac{B^2}{\beta} Q_2(p) \tag{5-10}$$

$$\frac{1}{4\pi}\int \varphi_T \, dv = \frac{B}{\beta^3} Q_4(p) \tag{5-11}$$

$$\frac{1}{4\pi}\int \varphi_T^3 \, dv = \frac{B^3}{\beta^3} Q_5(p) \tag{5-12}$$

The Q_i's are functions of the parameter, p, but the restriction

to a single parameter is not necessary. B and β are the other two parameters. Note that B, β, and p may not appear directly in the trial function (e.g. they may be combinations of the parameters of the trial function, such as $p = b/\alpha$.) The Lagrangian (4-1) will now be

$$L_T(B,\beta,p) = \frac{3}{2}\frac{B^2}{\beta^3}\left[Q_1(p) + \beta^2 Q_2(p) - \frac{B^2}{6} Q_3(p)\right] . \quad (5\text{-}13)$$

The two minimization equations,

$$\frac{\partial L_T}{\partial B} = 0 \quad \text{and} \quad \frac{\partial L_T}{\partial \beta} = 0 \ , \qquad (5\text{-}14)$$

demand that the following two relations hold:

$$B^2 = 3Q_1/Q_2 \qquad (5\text{-}15)$$

and

$$B^2 = 12Q_1/Q_3 \ . \qquad (5\text{-}16)$$

These values of β^2 and B^2 substituted into the special Lagrangian (5-13) yield

$$L_T = \frac{12Q_1Q_2}{Q_3}\sqrt{\frac{Q_2}{3Q_1}} \ . \qquad (5\text{-}17)$$

For a three parameter trial function, L_T is now a function of one parameter, the value of which is to be determined from the remaining extremization equation,

$$\frac{\partial L_T}{\partial p} = 0 \ . \qquad (5\text{-}18)$$

Alternately, a graph of the function $L_T(p)$ can be made, the extremums of L_T giving the solutions of equation (5-18). Usually,

L_T is a complicated function of p, so that the graphical method is quicker and easier to apply. When the above method of solving for the parameters has been used, the designation (OR1) will be placed beside the energy thus obtained.

If equations (5-15) and (5-16) are restored to their integral forms by using (5-8), (5-9), and (5-10), it is seen that the two integral relationships (5-4) and (5-5) are automatically satisfied.

The only other method of solving for the parameters that is used here is called (OR2) and is described below.

Suppose it is desired to have the integral condition (5-6) satisfied by the trial function. By using equation (5-11) and (5-12) it is seen that the integral condition may give a relation of the form,

$$B^2 = C_1(p) \quad . \tag{5-19}$$

A similar relation is always obtained from the orthogonality condition (5-7). This equation can be used in several ways together with the extremization conditions to determine the values of the parameters. The procedure (OR2) does the following. Substitute B^2 from (5-19) into the special Lagrangian, (5-13), reducing it to:

$$L_T(\beta,p) = \frac{3}{2}\,\frac{C_1(p)}{\beta^3}\left[\,\beta^2 Q_2(p) + C_2(p)\right.$$

where (5-20)

$$C_2 = Q_1 - C_1 Q_3/6 \ .$$

The extremization equation $\frac{\partial L_T}{\partial \beta} = 0$ gives,

$$\beta^2 = -3C_2/Q_2 \quad . \tag{5-21}$$

This value of β^2 used in (5-20) gives,

$$L_T = C_1 Q_2 \sqrt{\frac{-Q_2}{3C_2}} \quad . \tag{5-22}$$

L_T is again a function of a single parameter which can be determined as before.

The results for various trial functions follow:

1. Spherically symmetric solutions.

The accuracy of the numerical solution φ_0 was discussed in T. In all of this work with the V.M. it is assumed that the numerical solutions φ_0 and φ_1 are more exact than any of the trial functions. Thus, there are three spherically symmetric solutions with which to compare the results of the V.M. calculations. In this work only two of these solutions have been approximated by the V.M. A table of the spherically symmetric trial functions appears below. The integrals and additional information for the functions appears in Appendix E.

To show that the V.M. is giving reasonable numbers for the parameters, the functions 1S (OR1) and 9S (OR1) are plotted together with the numerical solutions φ_0 and φ_1 in Figures 7 and 8. Notice that the V.M. has determined the position of the node quite well for φ_1, even when using the simple trial function 9S.

The energy obtained by the V.M. is in all cases larger than the numerical value. This is to be expected for the solutions with no node where (OR1) has been applied, since (OR1) on

Table 4

Spherically Symmetric Trial Functions

Designation	Function	Energy in units of mc^2/G	Remarks
	No Nodes		
1S	$Ae^{-\alpha r}$	13.856 (OR1) 14.10 (OR2)	$\varphi_R = \pm\sqrt{3}$
2S	$Ae^{-\alpha(\lvert z\rvert+\rho)}$	19.6 (OR1)	cylindrical coordinates
3S	$Ae^{-\alpha(\lvert x\rvert+\lvert y\rvert+\lvert z\rvert)}$	22.9 (OR1)	rectangular coordinates
4S	$A\exp\left[-\alpha r^n\right]$	13.856 (OR1)	see Fig.10, $n = 1$
5S	$A(e^{-\alpha r}-e^{-\beta r})/r$	13.89 (OR2)	$\varphi_R = \pm\sqrt{3}$
6S	$Ae^{-\alpha r} + Be^{-\beta r}$	14.07 (OR2)	$\varphi_R = \pm\sqrt{3}$; $\varphi_T'(0) = 0$
7S	$A(1 + br)e^{-\alpha r}$	13.828 (OR1) 14.10 (OR2)	see Fig. 11 $\varphi_R = \pm\sqrt{3}$; gives $b = 0$
8S	$A\left[(e^{-r}-e^{-\alpha r})/r - \left(\frac{1-\alpha^2}{2\alpha}\right)e^{-\alpha r}\right]$	13.563 (OR1) 13.556 (OR2)	see Fig. 13 $\varphi_R = \pm\sqrt{3}$
	Teshima's solution; φ_0	13.53	
	One Node		
9S	$A(1 - br)e^{-\alpha r}$	89.745 (OR1) 89.57 (OR2)	see Fig. 12 $\varphi_R = \pm\sqrt{3}$
	Teshima's solution; φ_1	85.14	

Note : The (OR) following the energy refers to the method used for determining the parameters. See page 41 and 42.

Figure 7

The solid curve shows the first solution, φ_0, while the dashed curve is the approximation given by trial function 1S (OR1).

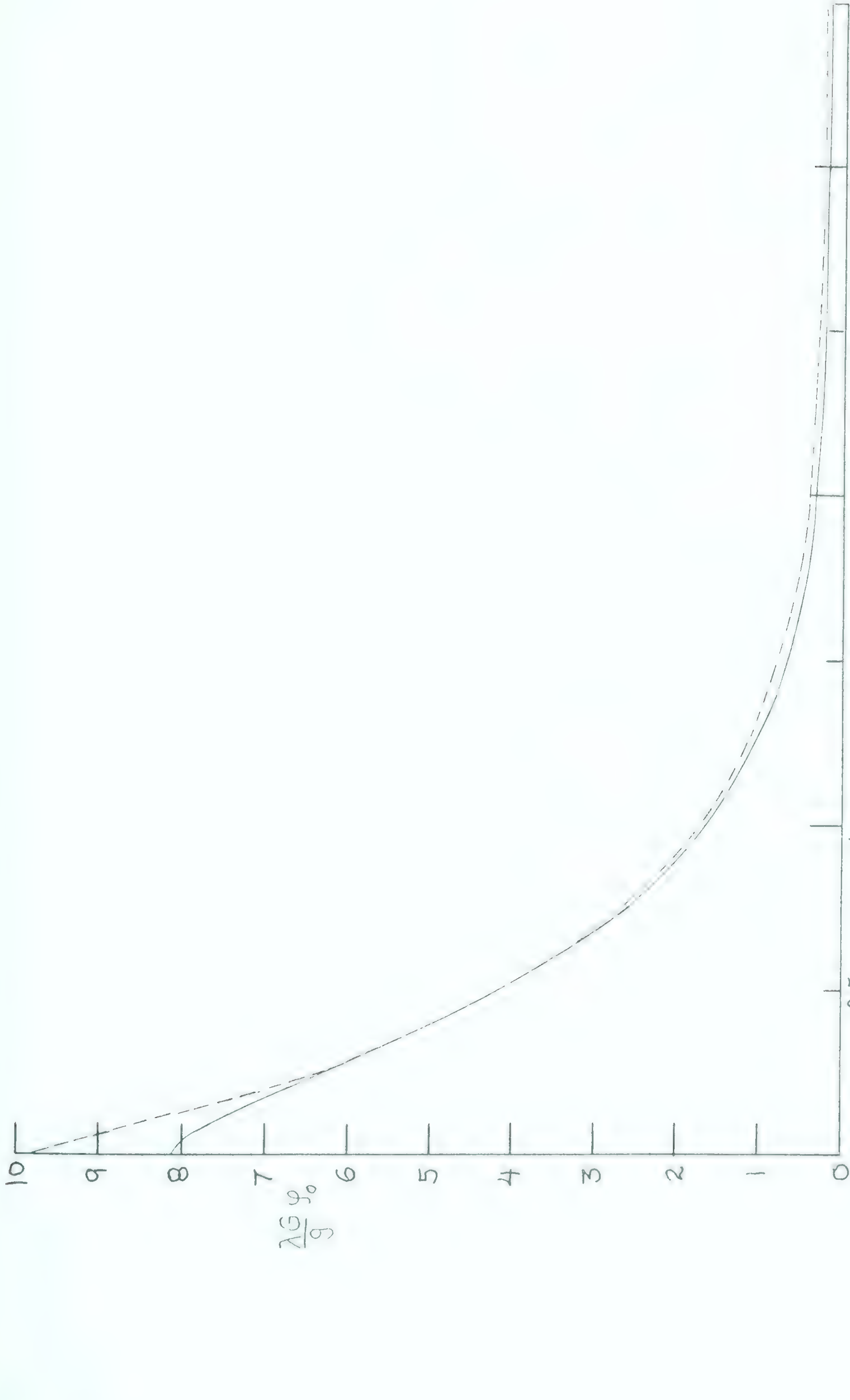

FIG. 7

Figure 8

The solid curve shows the second solution, φ_1, while the dashed curve is the approximate solution given by trial function 9S (OR1).

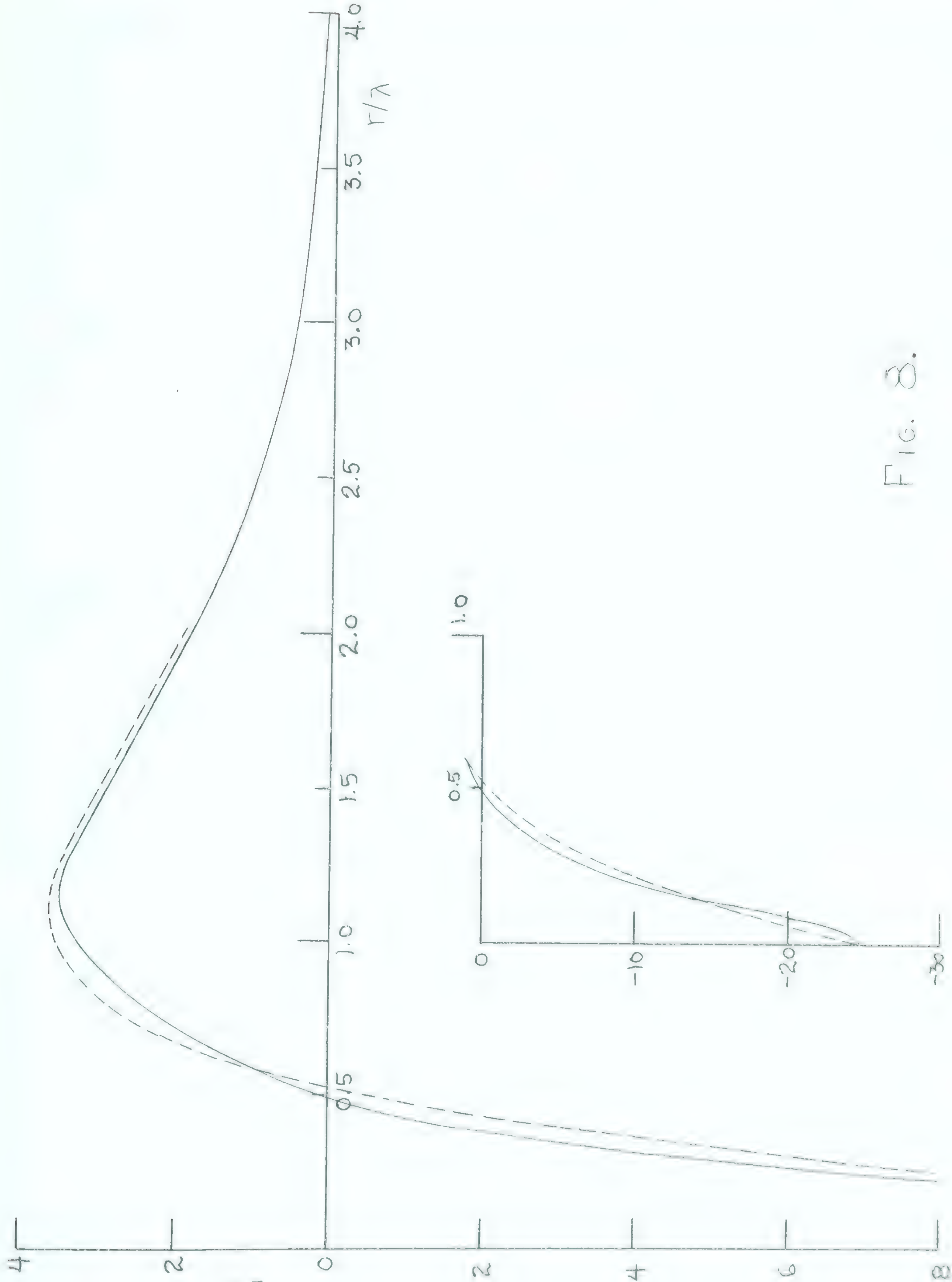

FIG. 8.

the Lagrangian (4-1) is equivalent to variational method I of Chapter IV. Note that (OR2) is not equivalent to any of the variational problems so that the energy given by this method may be above or below the exact value. The function 9S with one node also may not necessarily have definite bounds, since this function has not been made orthogonal to the nodeless solution which is the necessary condition for the results of variational problem III to apply.

Function 8S is the one obtained by using function 1S as the source density in the Green's function method of improving the trial functions. Note that this function has the correct asymptotic behaviour for large r together with a vanishing derivative at the origin. Since the (OR1) energy for this function is the lowest attained by any of the trial functions in Table 4 it is the "best" trial function. Table 5 shows a comparison of the numerical solution, φ_0, and the function 8S (OR1) for several values of the argument.

Table 5

Values of the Function 8S (OR1)
Compared to the Numerical Solution φ_0

r	$r\varphi_0$	$r\varphi_T$
0.064,538	0.478,246	0.515,511
0.133,531	0.951,270	1.004,643
0.207,639	1.379,875	1.426,423
0.287,682	1.727,586	1.755,891
0.374,693	1.969,127	1.981,116
0.470,003	2.095,005	2.100,417
0.575,364	2.110,628	2.119,786
0.693,147	2.031,695	2.050,540
0.826,678	1.878,421	1.907,208
0.980,829	1.670,884	1.705,666
1.163,151	1.426,316	1.461,554
1.386,294	1.158,129	1.188,985
1.673,976	0.876,012	0.899,585
2.079,442	0.586,523	0.601,898
2.772,589	0.293,757	0.301,231

2. Solutions of odd parity.

We shall try to approximate the eigensolution of equation (1-9) which is cylindrically symmetric, has odd parity, and only the one nodal surface required by its parity, assuming this solution to exist. Because of its parity, these solutions are automatically orthogonal to the spherically symmetric solutions so that orthogonalization is not required as a subsidiary condition and variational method I or II may be applied.

A table of the trial functions used appears below. Again, the integrals and parameter values for these functions are found in Appendix E. The table will not be discussed in detail since it is self explanatory.

Function 7P is obtained by using function 1P as the source density in the Green's function method of improving the trial functions. One would expect 7P to be quite a good approximation to the actual solution, similar to the situation that occured for the spherically symmetric solutions. However, the integral relationship, (4-5), is not satisfied by a factor of about two. If the numerical work is correct, this probably indicates that the original source function, 1P, is a very poor approximation to the actual solution.

If the $\cos\theta$ dependence of the trial functions is made more general, as in functions 6P and 8P, energies lower than the 49.26 of function 1P are obtained. The only minimum for function 8P is found for $n \longrightarrow \infty$. This seems to indicate that the field is concentrating itself in the x-y plane.

Trial function 9P is the difference of two spherically

Table 6

Odd Parity Trial Functions

Designation	Function	Energy in units of mc^2/G all (OR1)	Remarks
1P	$Ar\cos\theta e^{-\alpha r}$	49.26	
2P	$Ar\cos\theta e^{-\alpha(\rho+\|z\|)}$	52.1	cylindrical coordinates
3P	$Ar\cos\theta e^{-\alpha(\|x\|+\|y\|+\|z\|)}$	61.2	rectangular coordinates
4P	$Ar\cos\theta\ \exp\left[-\alpha r^n\right]$	42.5	see Fig. 14 gives $n \simeq 1.8$
5P	$A\ \cos\theta(e^{-\alpha r}-e^{-\beta r})$	49.26	reduces to function 1P
6P	$Ar\cos\theta(1+br^2\cos^2\theta)e^{-\alpha r}$	34.75	
7P	$\frac{A^3}{3}\left[\frac{3}{5}(\psi_1-\psi_3)\cos\theta + \psi_3\cos^3\theta\right]$	29.85	integral relationships poor. see Appendix C for ψ_1 and ψ_3
8P	$A(r\cos\theta)^{2n+1}\ e^{-\alpha r}$	32.0	see Fig. 15 $n \longrightarrow \infty$
9P	$A(e^{-\alpha r_1} - e^{-\alpha r_2})$	27.6	two spherical centres separated by a distance, s. see Fig. 16; $s \longrightarrow \infty$

symmetric functions such as 1S separated by a distance, s. The Lagrangian as a function of $2\alpha s$ is shown in Figure 16. The function L(s) has a minimum for $s = \infty$, since α approaches a constant for large s. Since the V.M. gives an upper bound, function 9P is the best solution of odd parity found so far.

These results seem to indicate that equation (1-9) has no single particle solution of odd parity.

3. Solutions with other types of spatial behaviour.

Only a few functions with symmetries other than those previously discussed have been tried. These are listed in Table 7 for reference only since most of them have not been investigated thoroughly.

Table 7

Trial Functions with Various Symmetries

Designation	Function	Energy in units of mc^2/G	Remarks
1H	$\psi_T = Ae^{-\alpha c\xi}$	13.8 (OR1)	Prolate spheroidal coordinates. $c \longrightarrow 0$; reduces to 1S.
2H	$\psi_T = Ae^{-\alpha c\xi}$	13.8 (OR1)	Oblate spheroidal coordinates. $c \longrightarrow 0$; reduces to 1S.
3H	$\psi_T = Ac^2\xi^2(3\eta^2-1)e^{-\alpha c\xi}$	118.24 (OR1)	$c \longrightarrow 0$; reduces to $\psi = Ar^2(3r^2 \cos^2\theta-1)e^{-\alpha r}$

Functions 1H and 2H are expressed in spheroidal coordinates and are therefore cylindrically symmetric. These functions were used in order to determine if the solution of lowest energy is spherically symmetric. The V.M. gives the reasonable result that the spheroid parameter, c, must be zero. Thus, functions 1H and 2H reduce to the nodeless spherically symmetric function 1S.

Function 3H is another spheroidal type function which was used to try to find a solution with symmetry similar to the D state solutions of the hydrogen atom. The spheroid parameter again was found to go to zero with the spheroidal coordinates reducing to spherical coordinates.

VI. Conclusion and Discussion

Since this non-linear theory is far from being comprehensive at the present time, we should not expect the masses of the particles as calculated by the theory to compare very well with the experimental results. In fact they do not. However, we have been able to show how particle like solutions may be found which possess definite mass ratios of the same order of magnitude as those occuring for the elementary particles. By assuming an expression for the interaction energy, it is possible to form various bound states of these fundamental particles. The coupling constant, G, also assumes the reasonable value of 13.53 if the energy of the first particle, φ_0, is taken to be mc^2.

The mathematical procedure of the variational method for the non-linear differential equation has been more rewarding. We have seen how the variational method may be used to find approximate analytic solutions of a non-linear differential equation. Furthermore, if the trial functions satisfy certain subsidiary conditions, the minimized Lagrangian will always furnish an upper bound to the energy. By use of this variational method quite accurate analytic expressions have been obtained for the first two spherically symmetric eigensolutions.

The variational method was used to try to find a solution of equation (1-9) with odd parity. The trial function of odd parity, giving the lowest energy so far, is the difference between two nodeless spherically symmetric functions. The two

spherical functions must be separated by an infinite distance to give the lowest energy. In effect we have found that equation (1-9) seems to have no single particle solution of odd parity.

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Appendix A: Proof of Integral Relationships

In this appendix we shall prove the following integral relationships holding for solutions of equation (1-9):

$$3\int \varphi dv = \int \varphi^3 dv \quad , \tag{A1}$$

$$3\int \left[\varphi + (\nabla\varphi)^2\right] dv = \int \varphi^4 dv \quad , \tag{A2}$$

$$12\int \varphi^2 dv = \int \varphi^4 dv \quad , \tag{A3}$$

$$3\int \varphi^2 dv = \int (\nabla\varphi)^2 dv \ , \tag{A4}$$

and if φ_1 and φ_2 are both solutions of equation (1-9),

$$\int \varphi_1\varphi_2^3 dv = \int \varphi_2\varphi_1^3 dv \quad . \tag{A5}$$

Integral relationship, (A3), was first noticed to hold for the numerical solutions of spherical symmetry and was proved analytically by Dr. H. Schiff for spherical symmetric solutions. It was thought it might fail for solutions of lower symmetry but Dr. D.D. Betts succeeded in proving it in general expressing the volume integrals in spherical coordinates. The following proof is carried out using the more compact vector notation.

Proof of (A1):

φ satisfies equation (1-9)

$$\nabla^2\varphi = \varphi - \frac{1}{3}\varphi^3 \tag{1-9}$$

Integrate both sides of this equation over all space. By Gauss' theorem,

$$\int_V \nabla^2\varphi dv = \oint_S \nabla\varphi \ dS$$

where the surface, S, bounds the volume, V. Since we consider only those solutions which are either zero or a constant at infinity, the surface integral is zero if the volume integral is over all space. Therefore,

$$\int(\varphi - \frac{1}{3}\varphi^3)dv = 0$$

which is (A1).

Proof of (A2):

Multiply (1-9) by φ and integrate over all space. By using Green's theorem,

$$\oint_S \varphi\nabla\varphi\cdot\vec{dS} - \int(\nabla\varphi)^2 dv = \int(\varphi^2 - \frac{1}{3}\varphi^4)dv \quad .$$

If φ is a constant or zero at infinity, the surface integral vanishes and equation (A2) follows.

Proof of (A3) and (A4):

Begin by integrating $\int\varphi^4 dv$ by parts:

$$\int\varphi^4 dv = -\frac{4}{3}\int\varphi^3(\vec{r}\cdot\nabla)\varphi dv$$

This relation can be proved by performing the integration by parts in rectangular coordinates. φ must also be zero at infinity, for the non integral term from the integration by parts to vanish. Now use equation (1-9) to replace the φ^3 term on the right giving,

$$\int\varphi^4 dv = -4\int\varphi(\vec{r}\cdot\nabla)\varphi dv + 4\int\nabla^2\varphi(\vec{r}\cdot\nabla)\varphi dv$$

After another integration by parts the first term on the right is $6\int\varphi^2 dv$. The second term may be transformed to

$$- 4 \int \nabla\varphi \cdot \nabla(\vec{r}\cdot\nabla)\varphi dv$$

by Green's theorem. Using the vector identity,

$$\nabla(\vec{u}\cdot\vec{v}) = \vec{u}\cdot\nabla\vec{v} + \vec{v}\cdot\nabla\vec{u} + \vec{u}x(\nabla x\vec{v}) + \vec{v}x(\nabla x\vec{u})$$

the integral becomes,

$$- 4\int \nabla\varphi\cdot \left[\vec{r}\cdot\nabla\nabla\varphi + \nabla\varphi\cdot\nabla\vec{r} + \vec{r}x(\nabla x\nabla\varphi) + \nabla\varphi x(\nabla x\vec{r})\right] dv$$

The last two terms are zero by virtue of the identities;

$$\nabla x\nabla\varphi = 0 \qquad \text{and} \qquad \nabla x\vec{r} = 0$$

The second integral is $- 4\int(\nabla\varphi)^2 dv$ since the del operator on the radius vector, $\vec{r}$, gives the unit dyadic. The first integral may be reduced by noting that

$$\nabla\varphi\cdot(\vec{r}\cdot\nabla\nabla\varphi) = \frac{1}{2}\,\vec{r}\cdot\nabla(\nabla\varphi)^2 \ .$$

This will give $6\int(\nabla\varphi)^2 dv$ after integrating by parts. Thus after collecting all the terms,

$$\int\varphi^4 dv = 2\int(\nabla\varphi)^2 dv + 6\int\varphi^2 dv \tag{A6}$$

If (A2) is now used the relations (A3) and (A4) result. Since Green's theorem as well as several integrations by parts have been used, φ must be zero at infinity for the surface integrals and constant terms arising from the integrations by parts to be zero.

Proof of (A5):

φ_1 and φ_2 both satisfy equation (1-9) thus:

$$\nabla^2\varphi_1 = \varphi_1 - \frac{1}{3}\varphi_1^3 \tag{A7}$$

$$\nabla^2 \varphi_2 = \varphi_2 - \frac{1}{3} \varphi_2^3 \tag{A8}$$

Multiply (A7) by φ_2, (A8) by φ_1, subtract and integrate over all space. Then by using the symmetric form of Green's theorem, the volume integrals containing the Laplacian reduce to surface integrals which are zero if φ_1 and/or φ_2 is zero or constant at infinity. The remaining integral is (A5).

Appendix B: Second Order Variational Terms

The Lagrangian (4-1) for a trial function, φ_1, is,

$$L_T = \frac{3}{8\pi}\int\left[\varphi_T^2 + (\nabla\varphi_T)^2 - \frac{1}{6}\varphi_T^4\right] dv$$

Now suppose $\varphi_T = \varphi + \epsilon f$, where φ is the actual solution of equation (1-9), ϵ is a small parameter, and f is an arbitrary function. For this φ_T, the Lagrangian up to terms of second order becomes,

$$L_T = \frac{3}{8\pi}\int\left[\varphi^2 + (\nabla\varphi)^2 - \frac{1}{6}\varphi^4\right] dv + \frac{3}{8\pi}\,\epsilon\int\left[2f\varphi + 2\nabla f\cdot\nabla\varphi - \frac{2}{3}\varphi^3 f\right] dv$$

$$\frac{3}{8\pi}\,\epsilon^2\int\left[f^2 + (\nabla f)^2 - \varphi^2 f^2\right] dv$$

The first term on the right is L, the Lagrangian for the actual solution. By using the fact that φ satisfies equation (1-9) and Green's theorem, the second term is zero. Thus L_T reduces to

$$L_T - L = \frac{3}{8\pi}\,\epsilon^2\int\left[f^2 + (\nabla f)^2 - \varphi^2 f^2\right] dv$$

This integral is not positive or negative definite for arbitrary f as can be seen by chosing $f = e^{-\alpha r}$ and using the fact that $\int \varphi^2 dv$ is bounded together with the Schwarz inequality. The sign of $L_T - L$ will depend on the value of α.

Appendix C: Results of Improving Odd Parity Trial Function by Means of Green's Function

Let us find the solution to the equation

$$\nabla^2\varphi - \varphi = -\frac{1}{3}\varphi_T^3$$

where $\varphi_T = Ar\cos\theta e^{-\alpha r}$; $A = 32$; $\alpha^2 = 3$.

The solution to

$$\nabla^2\varphi - \varphi = -4\pi\rho(r)$$

is given by

$$\varphi = \int G(r,r')\rho(r)dv$$

where $G(r,r') = \dfrac{e^{ik|r - r'|}}{|r - r'|}$; $k = i$

To perform the integration it is useful to use the expansion of $G(r,r')$ in spherical coordinates:

$$G(r,r') = ik \sum_{n,m} \epsilon_m (2n+1) \frac{(n-m)!}{(n+m)!} \cos m(\varphi - \varphi') P_n^m(\cos\theta) P_n^m(\cos\theta') \begin{cases} j_n(kr)h_n(kr'); & r \leq r' \\ j_n(kr')h_n(kr); & r \geq r' \end{cases}$$

Where:

P_n^m = Legendre functions of the first kind

j_n, h_n = spherical bessel functions

$\epsilon_m = 2; \quad m = 0$

$\quad = 1; \quad m \geq 1$

For the definition of these functions see Morse and Feshbach,

Methods of Theoretical Physics. φ is found in the form:

$$\varphi = \frac{A^3}{3}\left[\frac{3}{5}(\psi_1 - \psi_3)\cos\theta + \psi_3\cos^3\theta\right]$$

with

$$- 2 \times 10^3\psi_1 = (5.7950889)\left(\frac{r + 1}{r^2}\right)e^{-r} - \left(\frac{1}{r^2}\right)e^{-5.196r}\left[76.92777r^5 + 122.99723r^4 + 117.90271r^3 + 75.33156r^2 + 30.111282r + 5.7950889\right]$$

$$- 2 \times 10^3\psi_3 = (0.335965)\left(\frac{r^3 + 6r^2 + 15r + 15}{r^4}\right)e^{-r} - \left(\frac{1}{r^4}\right)e^{-5.196r}\left[76.92777r^7 + 122.99722r^6 + 147.49204r^5 + 146.29556r^4 + 115.20744r^3 + 67.524951r^2 + 26.185185r + 5.039490\right]$$

A graph of the functions ψ_1 and ψ_3 is found in Figure 9.

To calculate the energy for the improved trial functions we have:

$$\nabla^2\varphi - \varphi = -\frac{1}{3}\varphi_T^3$$

Multiply by φ, integrate over all space and use Green's theorem to give:

$$\int((\nabla\varphi)^2 + \varphi^2)dv = +\frac{1}{3}\int \varphi\varphi_T^3\, dv$$

The energy is given by

$$E = \frac{3}{8\pi}\int\left[(\nabla\varphi)^2 + \varphi^2 - \frac{1}{6}\varphi^4\right]dv$$

which can be reduced to

$$E = \frac{1}{8\pi}\int \varphi\varphi_T^3\, dv - \frac{1}{16\pi}\int \varphi^4 dv$$

by using the above relation. By numerical integration it was found:

Figure 9

The functions ψ_1, ψ_3, and $(\psi_1 - \psi_3)$ found by improving the odd parity function, $32r\cos\theta e^{-\sqrt{3}r}$, by a Green's function integration. The curves ψ_1, ψ_3, and $(\psi_1 - \psi_3)$ are labled on the graph.

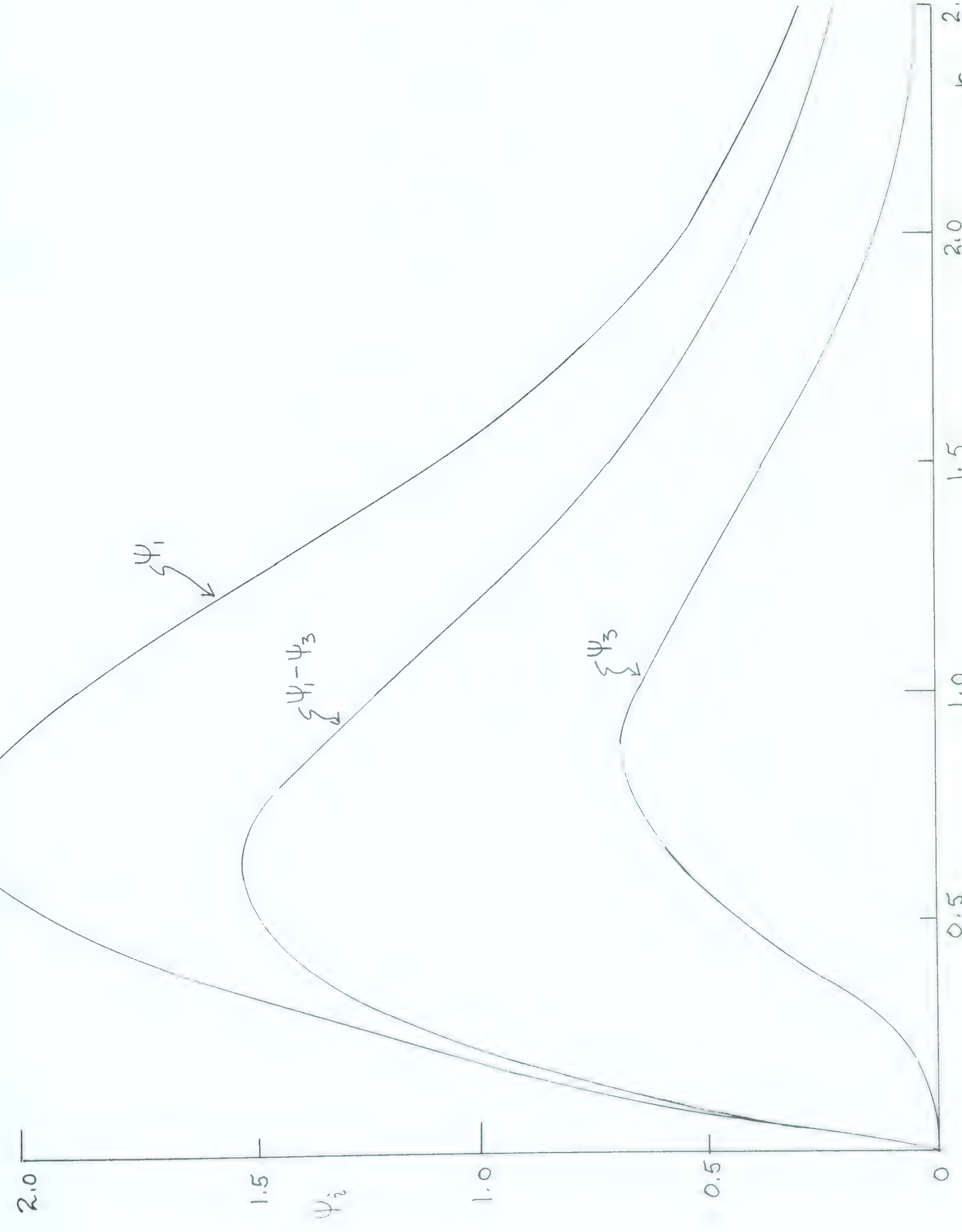

FIG. 9.

$$\frac{3}{4\pi}\int \varphi^2 dv = 49.452$$

$$\frac{1}{16\pi}\int \varphi^4 dv = 77.989$$

By direct integration:

$$\frac{1}{4\pi}\int \varphi\varphi_T^3 \, dv = 215.678$$

Therefore the energy is:

$$E = 107.839 - 77.989 = 29.85$$

Appendix D: Parameters for the Morse Potential Curves

The parameters for the three Morse potential curves shown in Figure 5 are given below.

$$V = V_0 \left[e^{-2(r-r_0)/a_0} - 2e^{-(r-r_0)/a_0} \right] \qquad (3\text{-}6)$$

curve	1	2	3
V_0	6.6	7.0	6.40
r_0	1.1	1.0	1.05
a_0	0.55	0.66	0.75

Appendix E: Integrals of the Trial Functions

With most of the trial functions used, the Lagrangian was reduced to a function of a single parameter with the function being evaluated numerically to determine the extrema. Therefore, most of the results are significant only to three figure accuracy. If the extrema have been found analytically the fact is stated in the "Results".

To simplify the notation the following abbreviations have been used:

$$P = \frac{1}{4\pi}\int \varphi_T^2 dv$$

$$Q = \frac{1}{4\pi}\int \varphi_T^4 dv$$

$$R = \frac{1}{4\pi}\int (\nabla\varphi_T)^2 dv$$

$$S = \frac{1}{4\pi}\int \varphi_T dv$$

$$T = \frac{1}{4\pi}\int \varphi_T^3 dv$$

$$L = P + R - \tfrac{1}{6}Q = L_T(\varphi_T)$$

E = value of L at minimum or maximum

1S; $Ae^{-\alpha r}$

$$P = \frac{A^2}{\alpha^3}\ \frac{1}{4}$$

$$Q = \frac{A^4}{\alpha^3}\ \frac{1}{32}$$

$$R = \frac{A^2}{\alpha}\ \frac{1}{4}$$

$$L = \frac{3}{2} \frac{A^2}{\alpha^3}\left[\frac{1}{4} + \frac{\alpha^2}{4} - \frac{1}{6(32)}A^2\right]$$

Results:

(OR1)

$E = 24/\sqrt{3} = 13.856$ analytically

$A^2 = 96$

$\alpha^2 = 3$

(OR2) $\varphi_R = \pm\sqrt{3}$

$E = 81/\sqrt{33} = 14.10$ analytically

$A = 9.0$

$\alpha = \sqrt{33}/4$

2S; $Ae^{-(\rho + |z|)}$

Cylindrical coordinates (ρ,θ,z) $\rho^2 = x^2 + y^2$

$$P = \frac{A^2}{\alpha^3} \frac{1}{8}$$

$$Q = \frac{A^4}{\alpha^3} \frac{1}{64}$$

$$R = \frac{A^2}{\alpha} \frac{1}{4}$$

$$L = \frac{3}{2} \frac{A^2}{\alpha^3}\left[\frac{1}{8} + \frac{\alpha^2}{4} - \frac{1}{6(64)}A^2\right]$$

Results:

(OR1)

$E = 19.6$ analytically

3S; $Ae^{-\alpha(|x| + |y| + |z|)}$

Rectangular coordinates (x,y,z)

$$P = \frac{A^2}{\alpha^3} \frac{1}{4\pi}$$

$$Q = \frac{A^4}{\alpha^3} \frac{1}{32\pi}$$

$$R = \frac{A^2}{\alpha} \frac{3}{4\pi}$$

$$L = \frac{3}{8\pi} \frac{A^2}{\alpha^3} \left[1 + 3\alpha^2 - \frac{1}{48} A^2\right]$$

Results:

(OR1)

$E = 22.9$ analytically

4S; $Ae^{-\alpha r^n}$

$$P = \frac{A^2}{n} (2\alpha)^{-3/n} \Gamma\left(\frac{3}{n}\right)$$

$$Q = \frac{A^4}{n} (4\alpha)^{-3/n} \Gamma\left(\frac{3}{n}\right)$$

$$R = n\alpha^2 (2\alpha)^{-\left(\frac{2n+1}{n}\right)} \Gamma\left(\frac{2n+1}{n}\right)$$

$$E^2 = \frac{9(n+1)^3 \Gamma^3(1+\frac{1}{n})}{4^{1-3/n} \Gamma(1+\frac{3}{n})}$$

$$A^2 = (12)\, 2^{3/n}$$

$$\alpha^{2/n} = \frac{3(4)^{n - 1/n} \Gamma(\frac{3}{n})}{n^2 \Gamma(\frac{2n+1}{n})}$$

Results:

See graph of E^2 vrs. n in Figure 10.

E = 13.8 at m = 1; minimum

5S; $A(e^{-\alpha r} - e^{-\beta r})/r$

Let $p = \beta/\alpha$; $B^2 = \alpha^2 A^2$

$$S = \frac{A}{\alpha^2}\left(\frac{p^2 - 1}{p^2}\right) = \frac{A}{\alpha^2}\, Q_4(p)$$

$$P = \frac{A^2}{\alpha}\, \frac{(p-1)^2}{2p(p+1)} = \frac{B^2}{\alpha^3}\, Q_1(p)$$

$$T = A^3 \left[\ln p + \ln\left(\frac{2+p}{1+2p}\right)^3 \right] = A^3 Q_5(p)$$

$$Q = 4\alpha A^4 \left[p \ln \left\{ \left(\frac{2p+2}{3p+1}\right)^3 \left(\frac{4p}{p+3}\right) \right\} - \ln \left\{ \left(\frac{p+3}{2p+2}\right)^3 \left(\frac{3p+1}{4}\right) \right\} \right]$$

$$= \frac{B^4}{\alpha^3}\, Q_3(p)$$

$$R = A^2 \alpha\, \frac{(p-1)^2}{2(p+1)} = \frac{B^2}{\alpha}\, Q_2(p)$$

Figure 10

The square of the Lagrangian as a function of the single parameter, n, for trial function 4S (OR1). The trial function is $Ae^{-\alpha r^{n}}$.

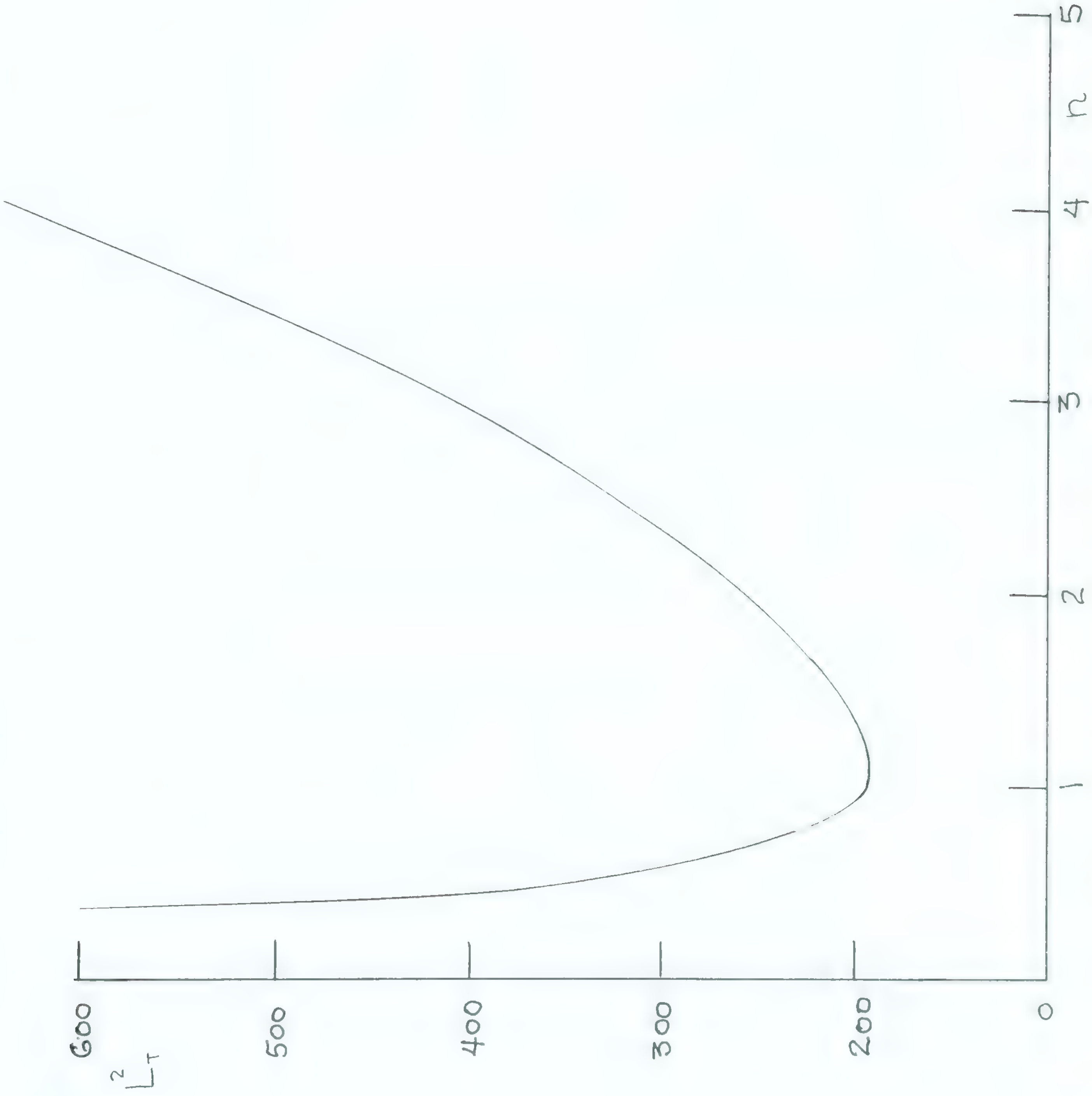

Fig. 10.

$$L = \frac{3}{2}\frac{B^2}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{B^2}{6}\,Q_3(p)\right]$$

Results:

(OR2) $\qquad\qquad \varphi_R = \pm\sqrt{3}$

$E = 13.897$

$A = 6.86$

$\alpha = 1.106$

$\beta = 2.582$

6S; $\quad Ae^{-\alpha r} + Be^{-\beta r}$ with $\frac{d\varphi_T}{dr} = 0$ at $r = 0$

Let $p = \beta/\alpha \qquad\qquad \alpha A + \beta B = 0$

$$S = \frac{2B}{\alpha^3}\left[\frac{1}{p} - p\right] = \frac{B}{\alpha^3}\,Q_4(p)$$

$$P = \frac{B^2}{\alpha^3}\frac{1}{4}\left[p^2 + \frac{1}{p^3} - \frac{16p}{(p+1)^3}\right] = \frac{B^2}{\alpha^3}\,Q_1(p)$$

$$T = \frac{B^3}{\alpha^3}\;\frac{2}{27}\left[\frac{1}{p^3} - p^3 + \frac{81p^2}{(p+2)^3} - \frac{81}{p^2(\frac{1}{p}+2)^3}\right] = \frac{B^3}{\alpha^3}\,Q_5(p)$$

$$Q = \frac{B^4}{\alpha^3}\;\frac{1}{32}\left[p^4 + \frac{1}{p^3} + \frac{48p^2}{(p+1)^3} - \frac{256p^2}{(p+3)^3} - \frac{256}{p^2(\frac{1}{p}+3)^3}\right] = \frac{B^4}{\alpha^3}\,Q_3(p)$$

$$R = \frac{B^2}{\alpha}\frac{1}{4}\left[p^2 + \frac{1}{p} - \frac{16p^2}{(p+1)^3}\right] = \frac{B^2}{\alpha}\,Q_2(p)$$

$$L = \frac{3}{2}\frac{B^2}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{B^2}{6}\,Q_3(p)\right]$$

Results:

(OR2) $\varphi_R = \pm\sqrt{3}$

$E = 14.07$

$B = 0.93$

$A = -8.95$

$\beta = 13.57$

$\alpha = 1.414$

7S, 9S; $A(1 \pm br)e^{-\alpha r}$

Let $p = b/\alpha$

$$S = \frac{A}{\alpha^3}\, 2(1 \pm 3p) = \frac{A}{\alpha^3}\, Q_4(p)$$

$$P = \frac{A^2}{\alpha^3}\,\frac{1}{4}(1 \pm 3p + 3p^2) = \frac{A^2}{\alpha^3}\, Q_1(p)$$

$$T = \frac{A^3}{\alpha^3}\,\frac{2}{27}(1 \pm 3p + 4p^2 \pm \frac{20}{9}\, p^3) = \frac{A^3}{\alpha^3}\, Q_5(p)$$

$$Q = \frac{A^4}{\alpha^3}\,\frac{1}{32}(1 \pm 3p + \frac{9}{2}\, p^2 \pm \frac{15}{4}\, p^3 + \frac{45}{32}\, p^4) = \frac{A^4}{\alpha^3}\, Q_3(p)$$

$$R = \frac{A^2}{\alpha}\,\frac{1}{4}(\, 1 \pm p + p^2) = \frac{A^2}{\alpha}\, Q_2(p)$$

$$L = \frac{3}{2}\,\frac{A^2}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{1}{6}\, B^2 Q_3(p)\right]$$

Results: See graphs of $I(p)$ in Figures 11 and 12.

7S; chose the plus sign:

(OR1)

$E = 13.828$

$\alpha = 2.27$

$A = 8.97$

$b = 0.908$

(OR2) $\varphi_R = \pm\sqrt{3}$

$E = 14.10$	$S = 6.0769$	$Q = 61.2197$
$\alpha = 1.436$	$P = 6.8365$	$R = 14.1003$
$A = 9.0$	$T = 18.2307$	
$b = 0.0$		

9S; chose the negative sign:

(OR1)

$E = 89.745$

$\alpha = 1.802,391$

$A = 24.904,94$

$b = 1.875,068$

(OR2) $\varphi_R = \pm\sqrt{3}$

$E = 89.57$	$S = -15.9922$	$Q = 337.2462$
$\alpha = 1.875$	$P = 26.3511$	$R = 89.5697$
$A = 25.70$	$T = -47.9767$	
$b = 1.970$		

Figure 11

The Lagrangian as a function of the single parameter, $p = b/\alpha$, for the trial function 7S (OR1). The trial function is $A(1+br)e^{-\alpha r}$.

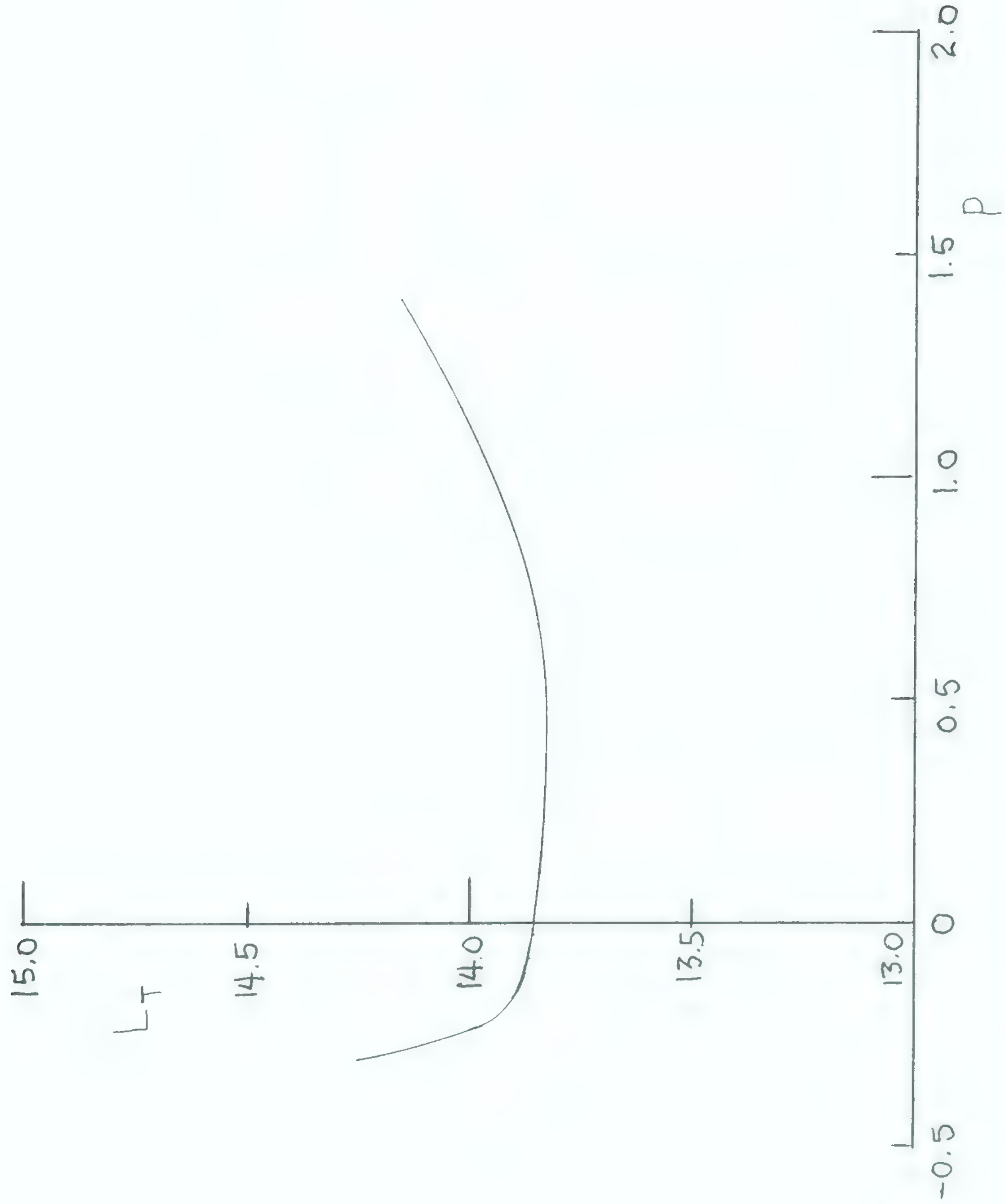

FIG. 11.

Figure 12

The Lagrangian as a function of the single parameter, $p = b/\alpha$, for the trial function 9S (OR1). The trial function is $A(1-br)e^{-\alpha r}$.

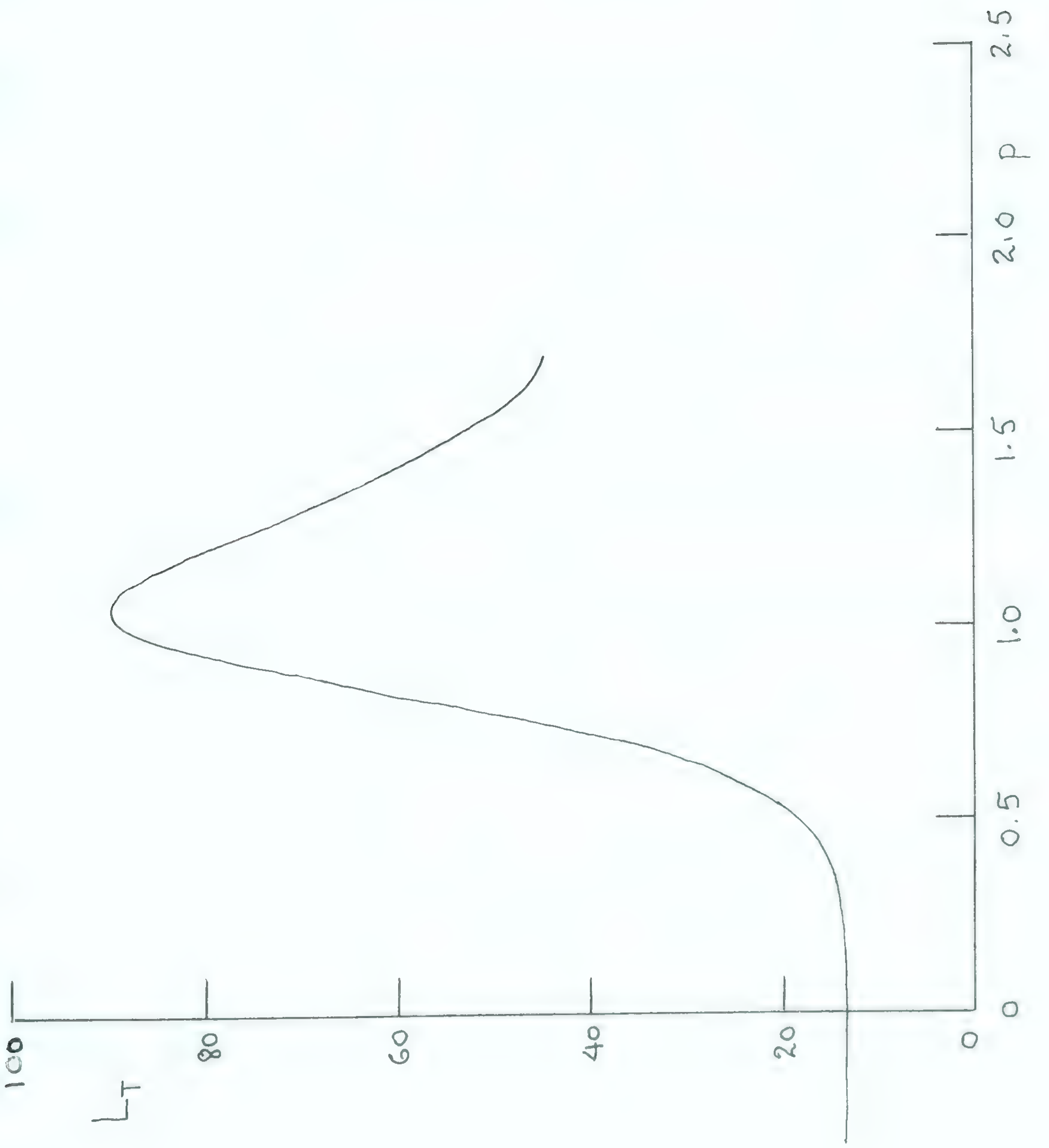

FIG. 12.

$$8S; \quad A\left[\frac{e^{-r} - e^{-\alpha r}}{r} - \left(\frac{\alpha^2 - 1}{2\alpha}\right)e^{-\alpha r}\right]$$

$$S = A\left(1 - \frac{2}{\alpha^2} + \frac{1}{\alpha^4}\right) = AQ_4(\alpha)$$

$$P = A^2\left(\frac{1}{2} + \frac{1}{16}\,\frac{1}{\alpha^5} - \frac{3}{8}\,\frac{1}{\alpha^3} + \frac{13}{16}\,\frac{1}{\alpha} - \frac{3}{\alpha + 1} + \frac{1}{\alpha(\alpha + 1)}\right) = A^2Q_1(\alpha)$$

$$T = A^3\left\{\ln\left[\alpha\left(\frac{\alpha + 2}{2\alpha + 1}\right)^3\right] + \left(\frac{1 - \alpha^2}{2\alpha}\right)\left(\frac{127}{108}\,\frac{1}{\alpha} - \frac{10}{54}\,\frac{1}{\alpha^3} + \frac{1}{108}\,\frac{1}{\alpha^5} + \right.\right.$$

$$\left.\left.\frac{3}{\alpha + 2} - \frac{6}{2\alpha + 1} + \frac{3}{2}\,\frac{(1 - \alpha^2)}{\alpha(2\alpha + 1)^2}\right)\right\} = A^3Q_5(\alpha)$$

$$Q = A^4\left\{2\left(\frac{\alpha^2 + 1}{\alpha}\right)\left[\ln\left(\frac{4\alpha}{\alpha + 3}\right)\left(\frac{2\alpha + 2}{3\alpha + 1}\right)^3\right] + 4\ln\left[\left(\frac{4}{3\alpha + 1}\right)\left(\frac{2\alpha + 2}{\alpha + 3}\right)^3\right] + \right.$$

$$\left(\frac{\alpha^2 - 1}{\alpha}\right)^2\left(\frac{209}{512}\,\frac{1}{\alpha} - \frac{9}{256}\,\frac{1}{\alpha^3} + \frac{1}{32}\,\frac{1}{\alpha^5} + \frac{3}{4}\,\frac{1}{\alpha + 1} - \frac{3}{3\alpha + 1} - \right.$$

$$\left.\left.\frac{1}{2}\,\frac{(\alpha^2 - 1)}{\alpha(3\alpha + 1)^2}\right)\right\} = A^4Q_3(\alpha)$$

$$R = A^2\left(\frac{3}{2} + \frac{1}{16}\,\frac{1}{\alpha^3} - \frac{7}{8}\,\frac{1}{\alpha} + \frac{5}{16}\,\alpha + \frac{1}{\alpha + 1} - \frac{3\alpha}{\alpha + 1}\right) = A^2Q_2(\alpha)$$

$$L = A^2\left[Q_1(\alpha) + Q_2(\alpha)\right] - \frac{A_4Q_3(\alpha)}{6}$$

$$\frac{\partial L}{\partial A} = 0 \text{ gives}$$

$$L = \frac{9}{4}\,\frac{\left[Q_1(\alpha) + Q_2(\alpha)\right]^2}{Q_3(\alpha)} \quad ; \quad A^2 = \frac{3\left[Q_1(\alpha) + Q_2(\alpha)\right]}{Q_3(\alpha)}$$

Results: See graph of $L(\alpha)$ for (OR2) in Figure 13.

(OR1)

$E = 13.563$ $\quad P = 4.5204$ $\quad R = 13.5634$

$\alpha = 5.20$ $\quad Q = 54.2515$

$A = 4.7453$

(OR2) $\quad \varphi_R = \pm\sqrt{3}$

$E = 13.556$ $\quad S = 4.35106$ $\quad Q = 51.8389$

$\alpha = 5.20$ $\quad P = 4.41874$ $\quad R = 13.2584$

$A = 4.6917$ $\quad T = 13.0532$

1P; $\quad Ar\cos\theta e^{-\alpha r}$

Let $\beta = 2\alpha$; $\quad B^2 = A^2/\beta^2$

$$P = \frac{A^2}{\beta^5}\,8$$

$$Q = \frac{A^4}{\beta^7}\,\frac{9}{8}$$

$$R = \frac{A^2}{\beta^3}\,2$$

$$L = \frac{3}{2}\,\frac{B^2}{\beta^3}\left[8 + 2\beta^2 - \frac{3}{16}\,B^2\right]$$

Figure 13

The Lagrangian as a function of the single parameter, α, for the trial function 8S (OR2). The trial function is

$$A\left[\frac{e^{-r}-e^{-\alpha r}}{r} + \left(\frac{1-\alpha^2}{2\alpha}\right)e^{-\alpha r}\right].$$

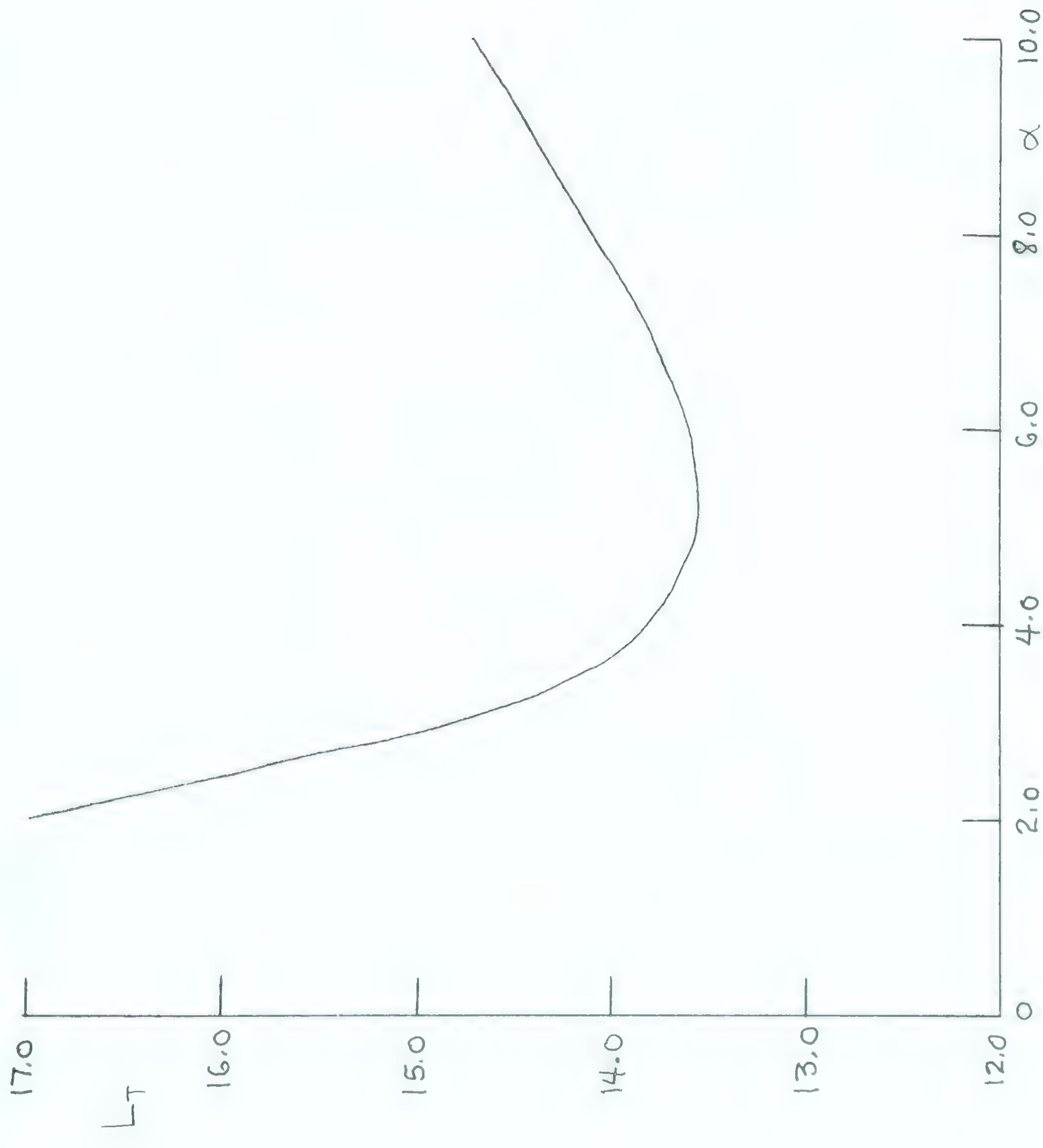

FIG. 13.

Results:

(OR1)

$E = 49.26$ analytically

$\alpha^2 = 3$

$A = 32$

2P; $Aze^{-\alpha(\rho + |z|)}$

Cyclindrical coordinates (ρ, θ, z); $\rho^2 = x^2 + y^2$

Let $B^2 = A^2/\alpha^2$

$$P = \frac{A^2}{\alpha^5} \frac{1}{16}$$

$$Q = \frac{A^4}{\alpha^7} \frac{3}{2048}$$

$$R = \frac{A^2}{\alpha^3} \frac{1}{8}$$

$$L = \frac{3}{2} \frac{B^2}{\alpha^3} \left[\frac{1}{16} + \frac{\alpha^2}{8} - \frac{1}{4096} B^2\right]$$

Results:

(OR1)

$E = 52.1$ analytically

3P; $Aze^{-\alpha(|x|+|y|+|z|)}$

Rectangular coordinates (x,y,z)

Let $B^2 = A^2/\alpha^2$

$$P = \frac{A^2}{\alpha^5}\frac{1}{8\pi}$$

$$Q = \frac{A^4}{\alpha^7}\frac{3}{1024\pi}$$

$$R = \frac{A^2}{\alpha^3}\frac{3}{8\pi}$$

$$L = \frac{3B^2}{8\pi\alpha^3}\left[\frac{1}{2} + \frac{3\alpha^2}{2} - \frac{1}{512}B^2\right]$$

Results:

(OR1)

$E = 61.2$ analytically

4P; $Ar\cos\theta e^{-\alpha r^n}$

$$P = \frac{A^2}{3}\frac{(2)^{-5/n}}{n} \quad \alpha^{-5/n}\Gamma\left(\frac{5}{n}\right)$$

$$Q = \frac{A^4}{5}\frac{(2)^{-14/n}}{n} \quad \alpha^{-7/n}\Gamma\left(\frac{7}{n}\right)$$

$$R = \frac{A^2}{4}\frac{(2)^{-3/n}}{n} \quad \alpha^{-3/n}\Gamma\left(\frac{3}{n}\right)$$

$$L = \frac{5}{2}(2)^{7/n}\ \frac{(n+3)^{3/2}}{n}\ \frac{\Gamma^{3/2}(\frac{3}{n})\ \Gamma^{1/2}(\frac{5}{n})}{\Gamma(\frac{7}{n})}$$

Results: See graph of $L(n)$, Figure 14.

A and α will be given by the two equations:

$$12\int \varphi_T^2 dv = \int \varphi_T^4 dv \quad \text{and} \quad 3\int \varphi_T^2 dv = \int (\nabla\varphi_T)^2 dv$$

(151)

$E = 42.5$

$n = 1.8$

5P; $A\cos\theta(e^{-\alpha r} - e^{-\beta r})$

Let $p = \beta/\alpha$

$$P = \frac{A^2}{\alpha^3}\frac{1}{12}\left[1 + \frac{1}{p^3} - \frac{16}{(p+1)^3}\right] = \frac{A^2}{\alpha^3} Q_1(p)$$

$$Q = \frac{A^4}{\alpha^3}\frac{1}{160}\left[1 - \frac{256}{(p+3)^3} + \frac{48}{(p+1)^3} - \frac{256}{(3p+1)^3} + \frac{1}{p^3}\right] = \frac{A^4}{\alpha^3} Q_3(p)$$

$$R = \frac{A^2}{\alpha}\frac{1}{12}\left[5 + \frac{5}{p} - \frac{16}{p+1} - \frac{16p}{(p+1)^3}\right] = \frac{A^2}{\alpha} Q_2(p)$$

$$L = \frac{3}{2}\frac{A^2}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{1}{6} A^2 Q_3(p)\right]$$

Figure 14

The Lagrangian as a function of the single parameter, n, for the trial function 4P. The trial function is $Ar\cos\theta e^{-\alpha r^n}$.

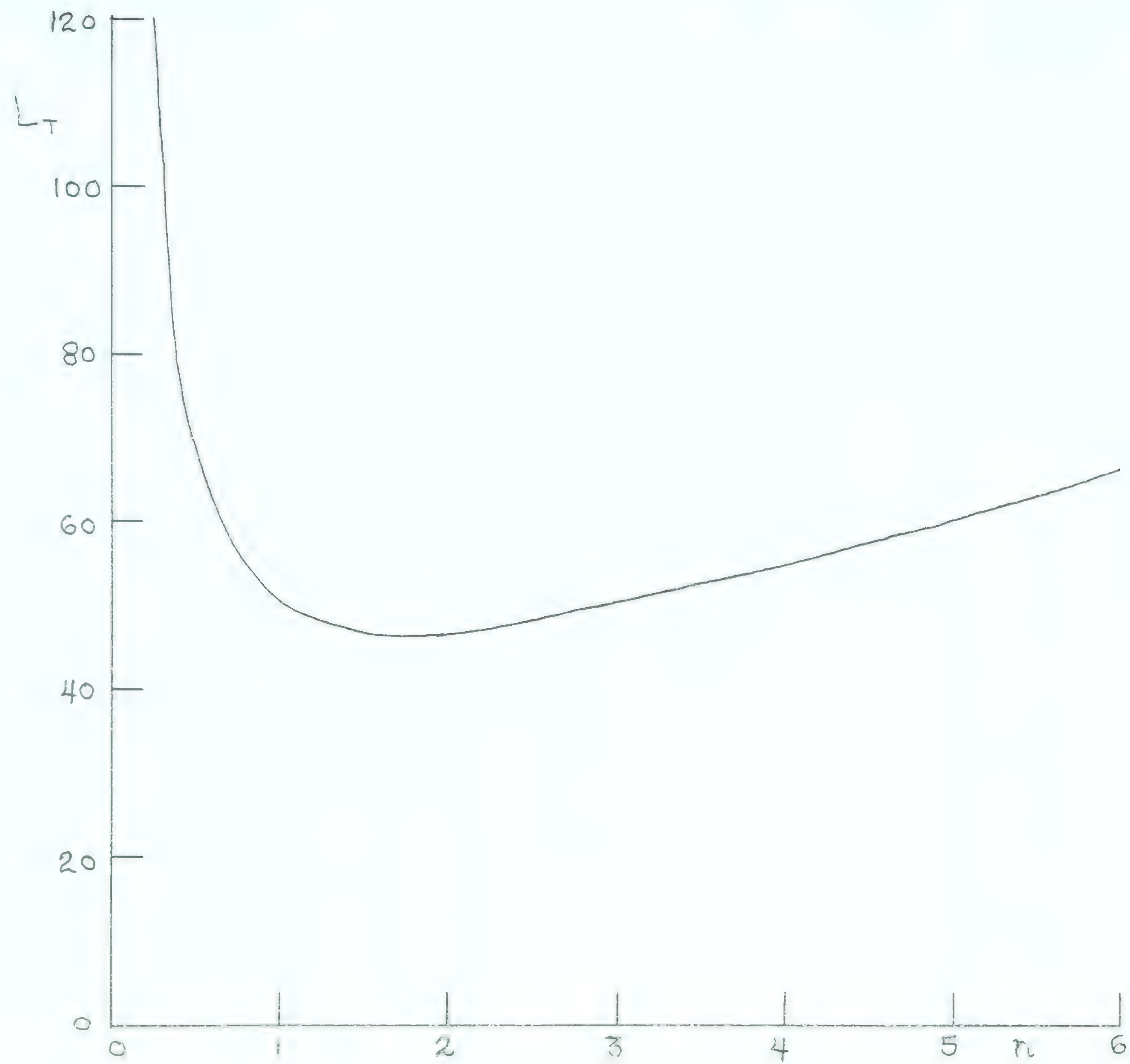

Fig. 14.

Results:

Found no extremum except near $p = 1$. At $p = 1$, $\alpha = \beta$ and φ_T reduces to:

$$\varphi_T = Ar\cos\theta e^{-\alpha r}$$

which is the function 1P.

Proof:

I_T is of the specialized form so that A will be given by:

$$A^2 = 12 \frac{Q_1(p)}{Q_3(p)}$$

Let $p = 1 + \epsilon$, then the Q's become:

$$Q_2 = \frac{\epsilon^2[24 + 24\epsilon + 5\epsilon^2]}{12[1 + \epsilon]^3[2 + \epsilon]^3}$$

$$Q_1 = \frac{\epsilon^2[24 + 48\epsilon + 33\epsilon^2 + 9\epsilon^3 + \epsilon^4]}{12[1 + \epsilon]^3[2 + \epsilon]^3}$$

$$Q_3 = \epsilon^4(46,080 + 184,320\epsilon + 306,240\epsilon^2 + 273,600\epsilon^3$$
$$+ 142,300\epsilon^4 + 43,440\epsilon^5 + 7,515\epsilon^6 + 675\epsilon^7$$
$$+ 27\epsilon^8)/(4 + \epsilon)^3(4 + 3\epsilon)^3(1 + \epsilon)^3(2 + \epsilon)^3$$

In the limit of $\epsilon \longrightarrow 0$ $\quad (p \longrightarrow 1)$

$$\lim_{\epsilon \to 0} A^2 = \frac{32^2}{\epsilon^2}$$

and

$$\lim_{\epsilon \to 0} \varphi_T = \lim_{\epsilon \to 0} A\cos\theta(1 - e^{-\epsilon r})e^{-\sqrt{3}r}$$

$$= \lim_{\epsilon \to 0} \frac{32}{\epsilon} \epsilon r\cos\theta e^{-\sqrt{3}r} = 32r\cos\theta e^{-\sqrt{3}r}$$

which is the function 1P.

6P, 5H; $Ar\cos\theta(1 \pm br^2\cos^2\theta)e^{-\alpha r}$

Let $p = b/\alpha^2$; $A^2 = \alpha^2 B^2$

$$P = \frac{A^2}{\alpha^5}\frac{1}{4}(1 \pm 9p + 45p^2) = \frac{B^2}{\alpha^3} Q_1(p)$$

$$Q = \frac{A^4}{\alpha^7}\frac{90}{2048}\left(\frac{1}{5} \pm 2p + \frac{105}{8}p^2 \pm \frac{945}{16}p^3 + \frac{72765}{512}p^4\right) = \frac{B^4}{\alpha^3} Q_3(p)$$

$$R = \frac{A^2}{\alpha^3}\frac{1}{4}(1 \pm 3p + 18p^2) = \frac{B^2}{\alpha} Q_2(p)$$

$$L = \frac{3}{2}\frac{B^2}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{1}{6}B^2 Q_3(p)\right]$$

Results:

Function 6P, chose the plus sign.

(CR1)

$E = 34.75$ $P = 11.5844$

$p = 1.36$ $Q = 139.013$

$\alpha = 2.746$ $R = 34.7531$

$A = 8.662$

Function 5H, chose the negative sign.

(CR1)

$E = 146.81$ $P = 48.9358$

$p = 0.207$ $Q = 587.2304$

$\alpha = 1.666$ $R = 146.8076$

$A = 48.61$

7P; $\frac{A^3}{3}\left[\frac{3}{5}(\psi_1 - \psi_3)\cos\theta + \psi_3\cos^3\theta\right]$

See Appendix C.

8P; $A(r\cos\theta)^{2n+1}e^{-\alpha r}$ $\qquad$ $n = 1,2,3\ldots$

Let $\beta = 2\alpha$; $B^2 = A^2(2\alpha)^{-4n-2}$

$$P = \frac{B^2}{\beta^3}\frac{(4n+4)!}{(4n+3)} = \frac{B^2}{\beta^3}Q_1(n)$$

$$Q = \frac{B^4}{(2)^{8n+7}\beta^3}\frac{(8n+6)!}{(8n+5)} = \frac{B^4}{\beta^3}Q_3(n)$$

$$R = \frac{B^2}{\beta}(4n+2)!\left[\frac{(2n+1)^2}{(4n+1)} - n\right] = \frac{B^2}{\beta}Q_2(n)$$

$$L = \frac{3}{2}\frac{B^2}{\beta^3}\left[Q_1(n) + \alpha^2 Q_2(n) - \frac{1}{6}\beta^2 Q_3(n)\right]$$

Results: See graph of $L(n)$ in Figure 15.

(OR1)

From the graph clearly the only extrema is for $n \longrightarrow \infty$. By using Stirling's approximation for the factorals in the above integrals it can be shown that:

$$\lim_{n\to\infty} L(n) = 18\sqrt{\pi}$$

$$\lim_{n\to\infty} \varphi_T(n) \longrightarrow \left[\frac{e^2(r\cos\theta)}{n^{1+1/n}\, e^{2r/\sqrt{n}}}\right]^n$$

where $e = 2.718\ldots$

Figure 15

The Lagrangian as a function of the single parameter, n, for the trial function 8P. The trial function is $A(r\cos\theta)^{2n+1}\ e^{-\alpha r}$.

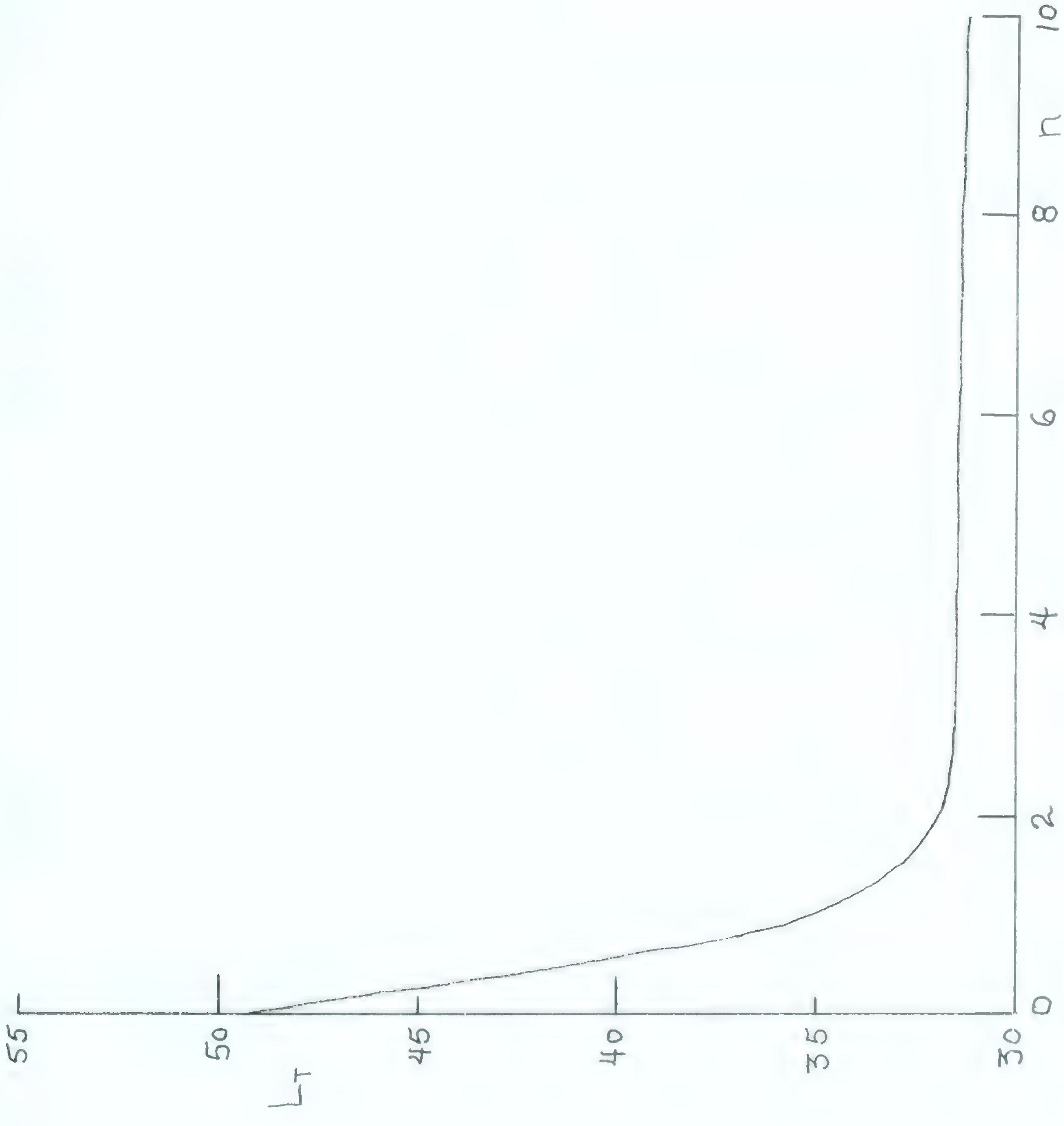

Fig. 15.

9P; $\psi_T = A(e^{-\alpha r_1} \pm e^{-\alpha r_2})$

Where $r_1^2 = r^2 + s^2 - 2rs\cos\theta$

$$r_2^2 = r^2 + s^2 + 2rs\cos\theta$$

s is a parameter which measures the separation of the two spherically symmetric systems. It is most convenient to use prolate ellipsoidal coordinates to perform the integrations.

Let $p = 2\alpha s$

$$P = \frac{A^2}{\alpha^3}\,\frac{1}{2}\left[1 \pm e^{-p}\left(\frac{p^2}{3} + p + 1\right)\right] = \frac{A^2}{\alpha^3}\,Q_1(p)$$

$$Q = \frac{A^4}{\alpha^3}\,\frac{1}{8}\left[\frac{1}{2} + e^{-2p}\left(2p^2 + 3p + \frac{3}{2}\right) \pm 3e^{-p}\left(2 - \frac{1}{p}\right) \pm e^{-3p}\left(2 + \frac{3}{p}\right)\right]$$

$$= \frac{A^4}{\alpha^3}\,Q_3(p)$$

$$R = \frac{A^2}{\alpha}\,\frac{1}{2}\left[1 \pm e^{-p}\left(\frac{-p^2}{3} + p + 1\right)\right] = \frac{A^2}{\alpha}\,Q_2(p)$$

$$L = \frac{3}{2}\,\frac{A^2}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{1}{6}\,A^2 Q_3(p)\right]$$

Results: See graph of L(p) in Figure 16.

1H; $Ae^{-\alpha c\xi}$

Prolate ellipsoidal coordinates defined by:

$$x = c\sqrt{(1 - \eta^2)(\xi^2 - 1)}\cos\varphi$$

Figure 16

The Lagrangian as a function of the single parameter, $p = 2\alpha s$, for the trial function 9P. The trial function is $A(e^{-\alpha r_1} - e^{-\alpha r_2})$.

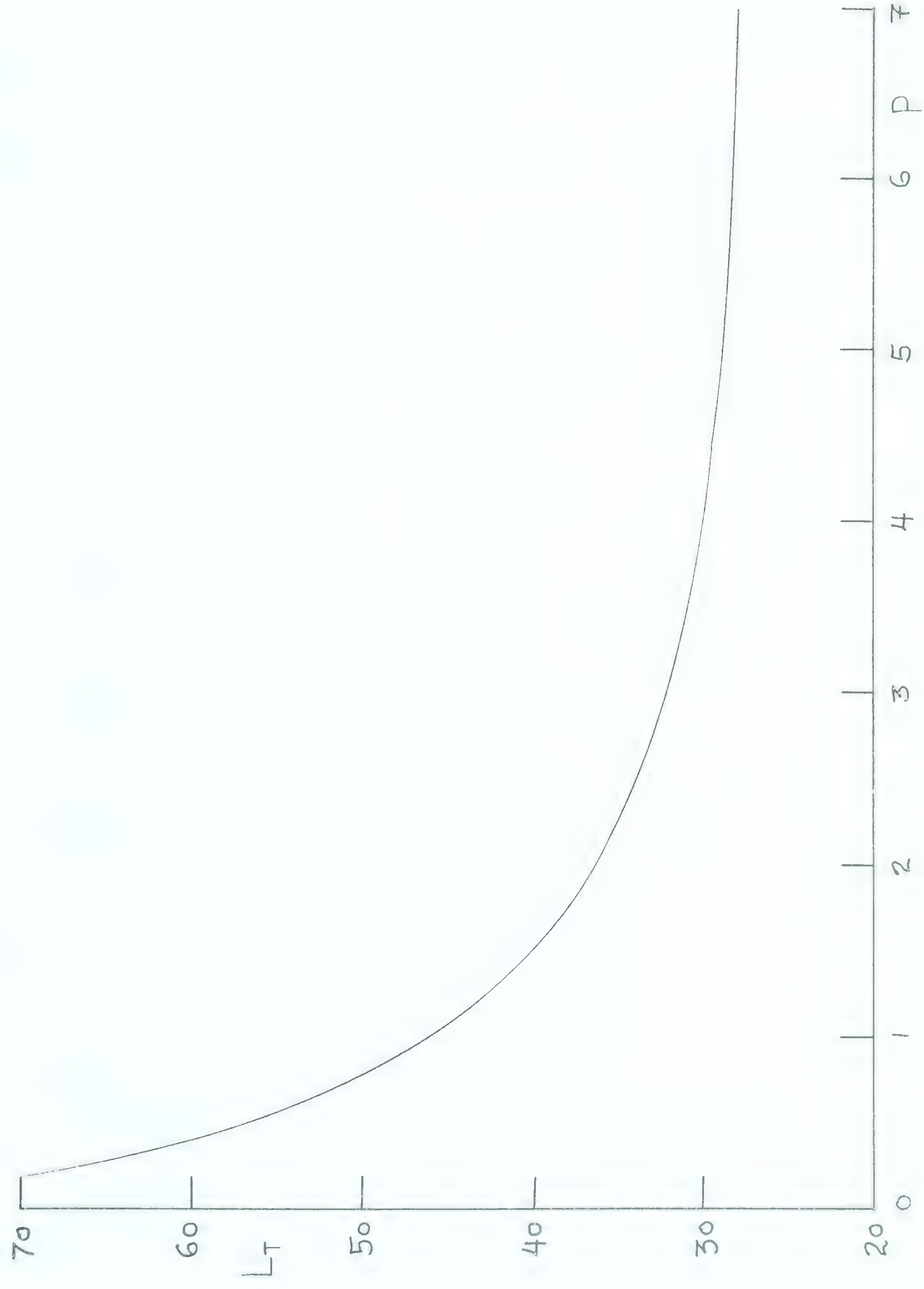

Fig. 16.

$$y = c\sqrt{(1 - \eta^2)(\xi^2 - 1)}\sin\varphi$$

$$z = c\xi\eta$$

Domain of the ξ, η, φ

$$-1 \leqslant \eta \leqslant +1$$

$$1 \leqslant \xi < \infty$$

$$0 \leqslant \varphi \leqslant 2\pi$$

Let $p = 2\alpha c$

$$S = \frac{A}{\alpha^3}\left[\frac{p^2}{6} + p + 2\right]e^{-p/2} = \frac{A}{\alpha^3}\,Q_4(p)$$

$$P = \frac{A^2}{\alpha^3}\left[\frac{p^2}{12} + \frac{p}{4} + \frac{1}{4}\right]e^{-p} = \frac{A^2}{\alpha^3}\,Q_1(p)$$

$$T = \frac{A^3}{\alpha^3}\left[\frac{p^2}{12} + \frac{p}{9} + \frac{2}{27}\right]e^{-3p/2} = \frac{A^3}{\alpha^3}\,Q_5(p)$$

$$Q = \frac{A^4}{\alpha^3}\left[\frac{p^2}{24} + \frac{p}{16} + \frac{1}{32}\right]e^{-2p} = \frac{A^4}{\alpha^3}\,Q_3(p)$$

$$R = \frac{A^2}{\alpha}\left[\frac{p}{4} + \frac{1}{4}\right]e^{-p} = \frac{A^2}{\alpha^3}\,Q_2(p)$$

$$L = \frac{3}{2}\,\frac{A^2}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{1}{6}A^2 Q_3(p)\right]$$

Results:

(OR1)

$E = 13.86$

The only real positive root to the equation $\frac{\partial L}{\partial p} = 0$ is

$p = 0$. When $p = 0$, $c = 0$ and $c\xi$ reduces to r. Therefore, this function reduces to 1S.

2H; $Ae^{-\alpha c\xi}$

Oblate ellipsoidal coordinates defined by:

$$x = c\sqrt{(1 - \eta^2)(1 + \xi^2)} \quad \cos\varphi$$

$$y = c\sqrt{(1 - \eta^2)(1 + \xi^2)} \quad \sin\varphi$$

$$z = c\xi\eta$$

Domain of the ξ, η, φ

$$-1 \leqslant \eta \leqslant +1$$

$$0 \leqslant \xi < \infty$$

$$0 \leqslant \varphi \leqslant 2\pi$$

Let $p = 2\alpha c$

$$P = \frac{A^2}{\alpha^3}\left[\frac{p^2}{24} + \frac{1}{4}\right] = \frac{A^2}{\alpha^3} Q_1(p)$$

$$Q = \frac{A^4}{\alpha^3}\left[\frac{p^2}{48} + \frac{1}{32}\right] = \frac{A^4}{\alpha^3} Q_3(p)$$

$$R = \frac{A^2}{\alpha}\left[\frac{p^2}{8} + \frac{1}{4}\right] = \frac{A^2}{\alpha} Q_2(p)$$

$$I = \frac{3}{2}\frac{A^3}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{1}{6} A^2 Q_3(p)\right]$$

Results:

(OR1)

$$E = 13.86$$

The only real positive root to the equation $\frac{\partial L}{\partial p} = 0$ is $p = 0$. When $p = 0$, $c = 0$ and $c\xi$ reduces to r. Therefore, this function reduces to 1S.

3H; $Ac^2\xi^2(3\eta^2 - 1)e^{-\alpha c\xi}$

Prolate ellipsoidal coordinates. See function 1H for definition.

Let $p = 2\alpha c$; $B^2 = A^2/\alpha^4$

$$P = \frac{A^2}{\alpha^7}\left[\frac{11}{35}\, p^2 + \frac{9}{2}\right] = \frac{B^2}{\alpha^3}\, Q_1(p)$$

$$Q = \frac{A^4}{\alpha^{11}}\left[\frac{8!}{2^{20}}\left(\frac{1168}{1155}\right) p^2 + \frac{10!}{2^{22}}\left(\frac{48}{35}\right)\right] = \frac{B^4}{\alpha^3}\, Q_3(p)$$

$$R = \frac{A^2}{\alpha^5}\left[\frac{p^2}{20} + \frac{9}{2}\right] = \frac{B^2}{\alpha}\, Q_2(p)$$

$$L = \frac{3}{2}\,\frac{B^2}{\alpha^3}\left[Q_1(p) + \alpha^2 Q_2(p) - \frac{1}{6}\, B^2 Q_3(p)\right]$$

Results:

(OR1)

$E = 107.03$

$p = 0$

The only real positive root to the equation $\frac{\partial L}{\partial p} = 0$ is $p = 0$, and therefore φ_T reduces to $Ar^2(3r^2\cos^2\theta - 1)e^{-\alpha r}$.

$Ar\cos\theta(1 - br)e^{-\alpha r}$

Let $p = b/\alpha$; $B^2 = A^2/\alpha^2$; $q = \alpha'/\alpha$

$$P = \frac{A^2}{\alpha^5}\frac{1}{4}\left[1 - 5p + \frac{15}{2}p^2\right] = \frac{B^2}{\alpha^3}Q_1(p)$$

$$Q = \frac{A^4}{\alpha^7}\frac{9}{1024}\left[1 - 7p + 21p^2 - \frac{63}{2}p^3 + \frac{315}{16}p^4\right] = \frac{B^4}{\alpha^3}Q_3(p)$$

$$R = \frac{A^2}{\alpha^3}\frac{1}{4}\left[1 - 3p + \frac{7}{2}p^2\right] = \frac{B^2}{\alpha}Q_2(p)$$

If $\varphi_R = A'r\cos\theta e^{-\alpha' r}$ then

$$\frac{1}{4\pi}\int \varphi_R^3\,\varphi_T\,dv = \frac{AA'^3}{\alpha^7}\frac{6!}{(3q + 1)^7}\left[1 - \frac{7p}{3q + 1}\right]$$

$$\frac{1}{4\pi}\int \varphi_R\,\varphi_T^3\,dv = \frac{A^3A'}{\alpha^7}\frac{6!}{(q + 3)^7}\left[1 - \frac{21p}{q + 3} + \frac{168p^2}{(q + 3)^2} - \frac{504p^3}{(q + 3)^3}\right]$$

Results:

(OR1)

$E = 161.29$	$P = 53.7647$
$A = 95.33$	$Q = 645.1761$
$\alpha = 1.744$	$R = 161.2940$
$b = 0.8764$	

(OR2) $\varphi_R = 32r\cos\theta e^{-\sqrt{3}r}$.

The two orthogonalization integrals above yield a relation $B^2 = C_1(p,q)$. A procedure identical to (OR2) reduces the

Lagrangian to a function of the two parameters p and q. A contour plot of $L_T(p,q)$ determines the parameter values.

E = 161.29	P = 53.7802
A = 95.426	Q = 646.0566
α = 1.744	R = 161.4245
b = 0.8766	

$A r\cos\theta(1 - br^2\cos^2\theta)e^{-\alpha r}$

See function 6P.

$A r\cos\theta e^{-\alpha r} + B r^3\cos^3\theta e^{-\beta r}$

Let $p = \frac{B}{A}\frac{1}{\alpha^2}$; $\lambda = \beta/\alpha - 1$; $C^2 = \frac{A^2}{\alpha^2}$

$$P = \frac{A^2}{\alpha^5}\, 12\left[\frac{1}{48} + \frac{24p}{(2+\lambda)^7} + \frac{15}{16}\frac{p^2}{(1+\lambda)^9}\right] = \frac{C^2}{\alpha^3}\, Q_1(p, \lambda)$$

$$Q = \frac{A^4}{\alpha^7}\, 360\left[\frac{1}{40960} + \frac{64p}{(4+\lambda)^9} + \frac{105p^2}{32(2+\lambda)^{11}} + \frac{483840p^3}{(4+3\lambda)^{13}} + \frac{72765}{4194304}\frac{p^4}{(1+\lambda)^{15}}\right] = \frac{C^4}{\alpha^3}\, Q_3(p, \lambda)$$

$$R = \frac{A^2}{\alpha^3}\, 2\left[\frac{1}{8} + \frac{24p}{(2+\lambda)^5} - \frac{24(4+\lambda)p}{(2+\lambda)^6} + \frac{144(1+\lambda)p}{(2+\lambda)^7} + \frac{9}{4}\frac{p^2}{(1+\lambda)^7}\right]$$

$$= \frac{C^2}{\alpha}\, Q_2(p, \lambda)$$

$$L = \frac{3}{2}\frac{C^2}{\alpha^3}\left[Q_1(p, \lambda) + \alpha^2 Q_2(p, \lambda) - \frac{1}{6}C^2 Q_3(p, \lambda)\right]$$

$A(u^n v^m - u^m v^n)e^{-\alpha(u + v)}$ $\qquad$ n,m integers

Parabolic coordinates defined by:

$$r = \frac{1}{2}(u + v)$$

$$z = \frac{1}{2}(u - v)$$

Let $\beta = 2\alpha$; $2n + 2m = k$

$$P = \frac{A^2}{(2\alpha)^{2n+2m+3}} \frac{(n + m + 1)}{2} \left[(2n)!\,(2m)! - (n + m)!^{\,2} \right] = \frac{A^2}{\beta^{k+3}} Q_1(n,m)$$

$$Q = \frac{A^4}{(4\alpha)^{4n+4m+3}} \frac{(2n + 2m + 1)}{2} \left[(4n)!\,(4m)! + 3(2n + 2m)!^{\,2} \right.$$

$$\left. - 4(3n + m)!\,(n + 3m)! \right] = \frac{A^4}{(2\beta)^{2k+3}} Q_3(n,m)$$

$$R = \frac{A^2}{(2\alpha)^{2n+2m+1}} \left[\frac{1}{2}(2n)!\,(2m)! + \frac{(n + m)!^{\,2}}{2} \left[\frac{(n - m)^2}{n + m} - 1 \right] \right]$$

$$= \frac{A^2}{\beta^{k+1}} Q_2(n,m)$$

$$L = \frac{3}{2} \frac{A^2}{\beta^{k+3}} \left[Q_1(n,m) + \beta^2 Q_2(n,m) - \frac{1}{6} \frac{Q_3(n,m)\,A^2}{(2)^{2k+3}\,\beta^k} \right]$$